UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	ANALIZA ZGRADBE KRISTALOV
Course Title:	CRYSTAL STRUCTURE ANALYSIS

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

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I02

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: izr. prof. dr. Amalija Golobič /
Dr. Amalija Golobič, Associate 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):
Osnovni principi zgradbe kristalov: Tipi vezi v kristalih (ionska, kovalentna, kovinska). Molekulska - Van der Waalsova vez, vodikova vez in druge interakcije med molekulami (npr. π...π in π...σ interakcije). Konkretni primeri kristalnih struktur za vsak tip vezi. Strukturni principi (koordinacijski poliedri in števila, elektrostatska jakost vezi, Paulingova pravila). Teoretične matematično-fizikalne osnove rentgenske strukturne analize: Povezanost položajev in intenzitete uklonov s strukturo urejene trdne snovi – z obliko in velikostjo osnovne celice ter njeno vsebino (položaji atomov v asimetrični enoti ter njihovi odmiki	Basic principles of crystal structure: Types of bonds (ionic, covalent, metal). Intermolecular interactions (Van der Waals, hydrogen bonds, π…π and π…σ stacking). Concrete examples of crystal structure for each type of bonding. Structural principles (coordination polyhedron and number, electrostatic bond strength, Pauling rules). Mathematical and physical fundamentals of X-ray structure analysis. The relationship between the position and intensity of reflections and the crystal structure (unit cell parameters, positional and displacement parameters of atoms in the asymmetric units and space group

od ravnovesnih leg in simetrije razporeditve atomov). Obnovitev pojmov: direktna in recipročna mreža, uklonski kot in indeksi uklonov, prostorska skupina. Uvedba novih pojmov: strukturni faktor, faza in amplituda uklonov, funkcija elektronske gostote, Lauejeva simetrija. Predstavitev faznega problema v kristalografiji ter njegovo reševanje, predvsem z metodo težkega atoma in direktnimi metodami. Izboljševanje oz. prilagajanje strukturnega modela. Interpretacija in analiza strukture. Predstavitev in uporaba kristalografskih baz anorganskih struktur (ICSD) ter Cambridge Structural database (CSD). Vaje: Opazovanje in prepoznavanje struktur ter ugotavljanje strukturnih podrobnosti s pomočjo računalniških programov za risanje in vizualizacijo in/ali s pomočjo gradnje tridimenzionalnih modelov. Študenti na osnovi prejetih uklonskih podatkov monokristala s pomočjo računalniških programov rešijo fazni problem, določijo strukturo ter jo narišejo in interpretirajo. S pomočjo ICSD ali CSD preverijo, ali je struktura že znana in poiščejo sorodne strukture. V primeru novih struktur lahko pripravijo rezultate za objavo v strokovni reviji.	symmetry). Recapitulation of conceptions: Direct and reciprocal lattice, diffraction angle, indices of reflections. New concepts: Structure factor, phase and amplitude of reflections, electron density function, Laue symmetry. A solution of a phase problem in crystallography (method of a heavy atom, direct methods), refinement of structural model, structure interpretation and analysis. Introduction and application of crystallographic databases: Inorganic crystal structure database (ICSD) and Cambridge structural database (CSD). Tutorial: Interpretation of crystal structures by using computer programs for drawing and visualization and/or by building of three-dimensional models. Small groups of students (by the help of teacher) perform the project of crystal structure determination and interpretation on the basis of single crystal diffraction data. They search for the same or similar structure in ICSD or CSD. In the case of novel crystal structure they can prepare structural results for the publication.

Temeljna literatura in viri / Readings:

1. W. Clegg: Crystal structure analysis: principles and practice. International Union of Crystallography, Oxford, New York : Oxford University Press, 2001, 265 pages.
2. W. Clegg: Crystal Structure Determination, Oxford Chemistry Primers, Oxford University Press, 2002, 87 strani.
3. U. Mueller: Inorganic Structural Chemistry, John Wiley & Sons, pp 36-60, 93-115, 146-183 of 264.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Razumevanje zgradbe anorganskih in organskih trdnih snovi ter strukturnih principov, ki jo določajo. Poznavanje principov uklanjanja rentgenskih žarkov na monokristalu. Kompetence: Določitev ter interpretacija strukture urejene trdne snovi na osnovi	*Objectives:* Knowledge of the structures of inorganic and organic solids and understanding of structural principles. Knowledge of principles of diffraction of X-rays on single crystals. *Competences:* Crystal structure determination and interpretation by single crystal X-ray diffraction data.

računalniške analize uklonskih podatkov monokromatske rentgenske svetlobe na monokristalu.	

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Razumevanje zgradbe organskih in anorganskih trdnih snovi ter strukturnih principov, ki jo določajo. Študent naj bi tudi razumel, kako je struktura kristala povezana z njegovo uklonsko sliko ter vedel, kako v praksi le-to uporabimo za določanje kristalnih struktur.	Knowledge and Comprehension Knowledge of the structures of inorganic and organic solids and understanding of structural principles. Comprehension of connection between crystal structure and its diffraction image. Crystal structure determination in practice.
Uporaba Študent pridobi osnovna znanja za strukturno analizo, se usposobi razumeti in interpretirati strukturni članek ter zna uporabljati podatke in orodja kristalografskih, strukturnih baz. Uri se v projektnem in timskem delu.	Application Basic knowledge of crystal structure determination. Capability of understanding and interpretation of crystallographic manuscripts. The application of tools and data from crystallographic structural databases. Training in project and team working.
Refleksija Zmožnost določitve in interpretacije eksperimentalne strukture v trdnem stanju pomaga razumeti in nudi možnost primerjave s strukturnimi rezultati drugih spektroskopskih tehnik in teoretičnih kvantno-kemijskih računov oziroma molekularne mehanike.	Analysis Capability of determination and interpretation of experimental structure of solids is helpful in understanding of structural results of spectroscopic techniques and quantum-chemical calculations or molecular mechanics.
Prenosljive spretnosti Projektno učno delo razvija samoiniciativnost študentov ter njihovo vključevanje v timsko delo. Veliko samostojnega dela z računalniškimi programi pripomore k študentovi spretnosti pri obvladovanju računalnika tudi pri drugih predmetih. Uporaba zbirk podatkov in literature, publiciranje rezultatov.	Skill-transference Ability Project work develops self-initiative of students and their comprehension in teamwork. Students get skills in working with computers. The application of databases and publishing of results.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**

- predavanja - praktične vaje v računalniški učilnici - projektno delo - individualne naloge	Lectures, tutorials in the computer classroom, project work and individual exercises.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit po uspešno opravljenem praktičnem delu. Ocene: 6-10 (pozitivno) in ocene 1-5: (negativno)		Written exam after successfully accomplished tutorials. - Grade: 6-10 (pozitive) and 1-5 (negative)

Reference nosilca / Lecturer's references:

1. **GOLOBIČ, Amalija***, ŠKAPIN, Srečo D., SUVOROV, Danilo, MEDEN, Anton. Solving structural problems of ceramic materials. *Croatica chemica acta*, ISSN 0011-1643, 2004, vol. 77, no. 3, str. 435-446.
2. **GOLOBIČ, Amalija***, MALEKOVIČ, Martina, ŠEGEDIN, Primož. Catena-poly[disodium [[diformatotricopper(II)]-di-[mu][sub]3-formato-tetra-[mu][sub]2-formato]] : a new mode of bridging between binuclear and mononuclear formate-copper(II) units. *Acta crystallographica. C, Crystal structure communications*, ISSN 0108-2701, 2006, vol. C62, no. 3, str. m102-m104.
3. KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, **GOLOBIČ, Amalija***. Structure of LaTi2Al9O19 and reanalysis of the crystal structure of La3Ti5Al15O37. *Acta crystallogr., B Struct. sci.*, 2011, vol. B67, no. 6, str. 455-460.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	ANORGANSKA KEMIJA
Course Title:	INORGANIC CHEMISTRY

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

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE211

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

Nosilec predmeta / Lecturer: prof. dr. Iztok Turel / Dr. Iztok Turel, Full Professor

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

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):
Predavanja: Uvod: soodvisnost strukture in kemijske vezi anorganskih spojin s- in p-elementov, spojin d-elementov, koordinacijskih in organokovinskih spojin. Vrste in mehanizmi anorganskih reakcij v koordinacijskih spojinah: izmenjava koordiniranih molekul topila, aktivacija molekul z interakcijo s kovinskimi ioni, homogena kataliza. Kemija elementov s poudarkom na zahtevnejših temah, ki niso bile zajete v Anorganski kemiji na 1. stopnji študija Kemije: kemija elementov 1., 2., 13.—18. skupine in prehodnih elementov.	**Lectures**: Introduction: the relations between chemical bond and the structure of inorganic compounds of s- and p-elements, compounds of d-elements, coordination and organometallic compounds. Mechanisms of reactions in coordination compounds, exchange of coordinated solvent molecules, activation of molecules by the interaction with metal ions, homogenous catalysis. Chemistry of the elements at advanced level and topics not covered in Inorganic Chemistry course at Bachelor level: Chemistry of the groups 1, 2, 13-18 and transition metals. **Seminar**: Determination of inorganic reaction mechanisms from activation entropy and

Seminar: Določanje mehanizma anorganskih reakcij iz aktivacijske entropije in aktivacijske prostornine, primeri študij izmenjave molekule vode kot liganda v raztopinah ionov prehodnih kovin. Metode za karakterizacijo anorganskih snovi in njihovih površin (elektronska mikroskopija, mikroskopija na atomsko silo, vrstična tunelska mikroskopija, rentgenska spektroskopija, elektronska spektroskopija, termična analiza). Koordinacijske spojine: primeri sinteze in kararakterizacije. Možne so tudi predstavitve nekaterih drugih aktualnih tem s področja anorganske kemije.	activation volume, examples of studies of exchange of water molecule ligands in solutions of transition-metal ions. Methods of characterization of inorganic substances and their surfaces (electron-, atom force-, scanning tunnelling microscopy, X-ray spectroscopy, thermal analysis). Coordination compounds: examples of syntheses and characterization. Presentations of certain other interesting topics from the field of inorganic chemistry are also possible.

Temeljna literatura in viri / Readings:

- C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, Second Edition, Pearson Education Limited, Harlow, England, 2005, 949 strani, poglavja 4, 6, 8, 18, 21-23, 25, 26 (skupaj 258 strani, 25%), knjiga dostopna v knjižnici FKKT.

Priporočena dodatna literatura:
- M. L Tobe, J. Burgess, Inorganic Reaction Mechanisms, Longman, Harlow, 1999, 674 strani.
-M. Weller, T. Overton, J. Rourke, and Fraser Armstrong, Inorganic Chemistry, Sixth Edition, Oxford University Press, Oxford, UK, 2014, 912 strani.

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta je nadgraditi znanje iz predmetov Splošna kemija in Anorganska kemija s teoretsko poglobljenim predmetom, ki podaja sintezo, reaktivnost, lastnosti in uporabo anorganskih snovi. *Kompretence:* razumevanje in načrtovanje zatevnejših anorganskih reakcij.	Objectives: to gain the in-deep understanding of principles of synthesis, reactivity, properties and application of inorganic compounds that are first coverd by General and Inorganic Chemistry courses in 1st Cycle. Competences: understanding and planning of advanced inorganic reactions.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Predmet predstavlja nadaljevanje predmetov Splošna in anorganska kemija I in II. Študent mora uporabiti znanja, ki jih je dobil pri osnovnih predmetih v prvih treh letnikih, da lahko osvoji vsebino (točka 14) tega predmeta.	<u>Knowledge and Comprehension</u> Understanding of advanced principles of the properties and reactivity of inorganic compounds Ability to understand and plan the syntheses of inorganic compound.
<u>Uporaba</u> Študent dobi poglobljeno teoretsko znanje, ki mu pomaga pri načrtovanju sintez spojin in predvidevanju njihovih lastnosti. Sposoben naj bi bil uporabljati svoje znanje	<u>Application</u> The students get the theoretical knowledge that help them to plan the synthesis of compounds and predict their properties. The students should be able to solve interdisciplinary

interdisciplinarno in na praktičnih primerih.	problems that involve inorganic chemistry.
Refleksija Kemija je eksperimentalna veda in osnovni cilj solidnega teoretskega znanja naj bo njegova uporaba.	Analysis Chemistry is experimental science and the goal of theoretical knowledge and theoretical research is its practical use.
Prenosljive spretnosti Predmet širi znanje in nakazuje interdisciplinarnost večine raziskovalnih in razvojnih dejavnosti.	Skill-transference Ability The course broadens the knowledge and shows the interdisciplinary nature of most research projects.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predmet se izvaja v obliki predavanj in seminarjev, pri katerih se snov poglobi in se obravnavajo aktualne teme s področja predmeta. Pri predavanjih se občasno uporabljajo tudi nekatere sodobnejše tehnike (študij primerov, uporaba računalniških in video predstavitev, ipd.).	Lectures and seminars. The seminars covers some experimental methods in inorganic chemistry: the background of the methods is described, the students observe the measurement and evaluate raw experimental data.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni in ustni izpit: ocene od 6-10 (pozitivno) oz. 1-5 (negativno).		Written and oral exam: 6-10 (pass the exam) and 1-5 (not pass the exam).

Reference nosilca / Lecturer's references:

- SERŠEN, Sara, KLJUN, Jakob, KRYEZIU, Kushtrim, PANCHUK, Rostyslav, ALTE, Beatrix, KÖRNER, Wilfried, HEFFETER, Petra, BERGER, Walter, **TUREL, Iztok**. Structure-related mode-of-action differences of anticancer organoruthenium complexes with ß-diketonates. Journal of medicinal chemistry, ISSN 0022-2623, 2015, vol. 58, iss. 9, str. 3984-3996, ilustr. http://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.5b00288, doi: 10.1021/acs.jmedchem.5b00288. [COBISS.SI-ID 1536265667]
- KLJUN, Jakob, BRATSOS, Ioannis, ALESSIO, Enzo, PSOMAS, George, REPNIK, Urška, BUTINAR, Miha, TURK, Boris, **TUREL, Iztok**. New uses for old drugs : attempts to convert quinolone antibacterials into potential anticancer agents containing ruthenium. Inorganic chemistry, ISSN 0020-1669, 2013, vol. 52, no. 15, str. 9039-9052, ilustr. http://pubs.acs.org/doi/pdf/10.1021/ic401220x, doi: 10.1021/ic401220x. [COBISS.SI-ID 1610287]
- SERŠEN, Sara, KLJUN, Jakob, POŽGAN, Franc, ŠTEFANE, Bogdan, **TUREL, Iztok**. Novel organoruthenium(II) ß-diketonates as catalysts for ortho arylation via C-H activation. Organometallics, ISSN 0276-7333, 2013, vol. 32, issue 2, str. 609-616. http://pubs.acs.org/doi/pdf/10.1021/om3011189, doi: 10.1021/om3011189. [COBISS.SI-ID 36426757]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	BIOFIZIKALNA KEMIJA
Course Title:	BIOPHYSICAL CHEMISTRY

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

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I21

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	**15**	**15 LV**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: prof. dr. Jurij Lah / Dr. Jurij Lah, Full 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):**
Biološko pomembne molekule Proteini, nukleinske kisline, polisaharidi, lipidi, maščobe, surfaktanti. Struktura, funkcija in njihovo okolje v celici .	**Biologically important molecules** Proteins, nucleic acids, polysaccharides, fats, lipids, surfactants. Structure, function and their environment in the cell.
Proteini, nukleinske kisline in lipidi v vodni raztopini Voda : Vodikove vezi , struktura ledu in tekoče vode. Hidratacija: Bornov model hidratacije ionov, solvatacija polarnih in nepolarnih topljencev, hidrofobni efekt. Interakcije, ki stabilizirajo strukturo proteinov in nukleinskih kislin. Proteini in nukleinske kisline kot polielektroliti. Topnost in kristalizacija proteinov. Tvorba in funkcija bioloških membran.	**Proteins, nucleic acids and lipids in aqueous solution** Water: Hydrogen bonds, structure of crystalline and liquid water. Solvation: The Born model of ion salvation, solvation of polar and non-polar solutes. The hydrophobic effect. Interactions stabilizing protein and nucleic acids structure. Proteins and nucleic acids as polyelectrolytes. Protein solubility and crystallization. Form and function of biological membranes.
Termodinamika biomolekularnih sistemov	**Thermodynamics of biomolecular systems**

Energija, informacije in življenje. Termodinamska analiza fotosinteze, glikolize, cikla citronske kisline, oksidativne fosforilacije in hidrolize ATP, osmoze, dialize, membranskega transporta, stabilnosti proteinov in nukleinskih kislin. Termodinamika medsebojnega prepoznavanja bioloških makromolekul : osnove, uporaba pri načrtovanju zdravil. **Kinetika** Hitrost reakcije in njena odvisnost od temperature. Mehanizmi zvitja in vezanja proteinov in nukleinskih kislin. Napačno zvitje proteinov in s tem povezane bolezni. Tehnike za spremljanje zelo hitrih procesov, relaksacijske metode, izmenjava vodika, površinska plazmonska resonanca.	Energy, information, and life. Thermodynamic analysis of photosynthesis, glycolysis, and the citric acid cycle, oxidative phosphorylation and ATP hydrolysis, osmosis, dialysis, membrane transport, protein stability and nucleic acids stability. Thermodynamics of recognition of biological macromolecules: introduction, application in drug design. **Kinetics** Rate of reaction and its temperature dependence. Mechanisms of protein and nucleic acids folding and binding. Protein folding and pathological misfolding. Rapid reaction techniques, relaxation methods, hydrogen exchange, surface plasmon resonance.

Temeljna literatura in viri / Readings:

- *Principles of Physical Biochemistry*, K.E. van Holde Prentice Hall (1998), 657 str., (30 %)
Biophysical Chemistry, A. Cooper, RSC, Cambridge (2004), 184 str., (50%)

Dopolnilna literatura:

- *Thermodynamics and Kinetics for the Biological Sciences*, G.G. Hammes, J. Wiley & Sons (2000), 158 str.

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta: Spoznavanje, razumevanje in obravnava fizikalno-kemijskih lastnosti bioloških makromolekul ter zakonitosti, ki te lastnosti določajo in povezujejo. *Predmetno specifične kompetence*: Sposobnost osnovne fizikalno-kemijske karakterizacije raztopin bioloških makromolekul, njihovega vezanja in strukturnih sprememb.	Knowledge and understanding of the basic physico-chemical properties of biological macromolecules in solution and understanding of physical laws that determine these properties and link them together. Ability to accomplish basic physico-chemical interpretation of properties of biological macromolecules in the solution, their binding and structural alterations.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Predmet daje študentu teoretično (predavanja, seminar) in praktično (laboratorijske vaje) znanje iz osnov biofizikalne kemije. Pridobljeno znanje je nujno potrebno pri razumevanju osnov termodinamike biokemijskih procesov na	<u>Knowledge and Comprehension</u> The subject gives students the theoretical (lectures, seminars) and practical (lab exercises) knowledge of basic biophysical chemistry. The acquired knowledge is necessary to understand basics thermodynamics of biochemical processes at the molecular level.

molekularnem nivoju.	
Uporaba Pridobljeno teoretično in praktično znanje je potrebno ne samo za uspešen študij drugih predmetov na magistrski stopnji ampak tudi za uspešno teoretično in praktično raziskovalno delo na področju biokemije.	Application Acquired theoretical and practical knowledge is necessary not only for successful study of other subjects at the MSc level but also for a successful theoretical and practical research in the field of biochemistry and chemistry.
Refleksija Študent bo pridobil občutek, kako s pomočjo osnov termodinamike lahko opišemo relativno zapletene biokemijske procese. S pridobljenim znanjem bo lahko kritično ovrednotil rezultate laboratorijskih vaj in ga uporabil v praksi.	Analysis Students will find out how to use thermodynamics in description of relatively complex biochemical processes. With the knowledge gained they will be able to critically evaluate the results of laboratory work and use it in biochemical and chemical practice.
Prenosljive spretnosti Študent se nauči nekaterih teoretičnih in eksperimentalnih pristopov, ki so osnova pri načrtovanju, spremljanju in vodenju eksperimentov v biokemiji.	Skill-transference Ability Students will learn some of the theoretical and experimental approaches, which set the basis for planning and monitoring experiments in biochemistry and chemistry.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji: z uporabo različnih učnih pripomočkov (kreda in tabla, Power Point, prosojnice). Vaje: skripta, teoretična navodila in praktične laboratorijske vaje.	Lectures, seminars, laboratory exercises.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit po uspešno opravljenih laboratorijskih vajah.		Written examination after successful completion of laboratory exercises.

Reference nosilca / Lecturer's references:

- Lah, J., Drobnak, I., Dolinar, M., Vesnaver, G. What drives the binding of minor groove-directed ligands to DNA hairpins?. *Nucleic Acids Res.*, **2008**, *36*, 897-904.

- Lah, J., Šimić, M., Vesnaver, G., Marianovsky, I., Glaser, G., Engelberg-Kulka, H., Loris, R. Energetics of structural transitions of the addiction antitoxin MazE. Is a programmed bacterial cell death dependent on the intrinsically flexible nature of the antitoxins?. *J. Biol. Chem.*, **2005**, *280*, 17397-17407.

- Lah, J., Bešter-Rogač, M., Perger, T. M., Vesnaver, G. Energetics in correlation with structural features: the case of micellization. *J. Phys. Chem, B* **2006**, *110*, 23279-23291.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	EKSPERIMENTALNA FIZIKALNA KEMIJA
Course Title:	EXPERIMENTAL PHYSICAL 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, 2nd Cycle	/	1st	2nd

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I17

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	20	25 LV	/	/	75	5

Nosilec predmeta / Lecturer: prof. dr. Jurij Lah / Dr. Jurij Lah, Full Professor
doc. dr. Janez Cerar / Dr. Janez Cerar, Assistant Professor
izr. prof. dr. Matija Tomšič / Dr. Matija Tomšič, Associate 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):
Izotermna kalorimetrija Fizikalne osnove signala, merjenje in analiza signala, razredčilna toplota, titracije, uporabnost pri študiju vezanja molekul. **Diferenčna dinamična kalorimetrija** Fizikalne osnove signala, merjenje in analiza signala, uporabnost pri študiju strukturnih sprememb makromolekul. **Spektropolarimetrija** Polarizirana svetloba, molekularne osnove signala, merjenje in analiza signala, titracije, uporabnost pri študiju (inducirane) asimetrije molekul.	**Isothermal calorimetry** Physical basics of the signal, measurement and analysis of the signal, heat of dilution, titrations, usefulness in the study of the molecular binding. **Differential scanning calorimetry (DSC)** Physical basis of the signal, measurement and analysis of the signal, usefulness in the study of structural changes of macromolecules. **CD-spectroscopy** Polarized light, circular dichroism (CD), molecular basis of the signal, measurement and signal analysis, CD - titration usefulness in the

Fluorimetrija Molekularne osnove signala, merjenje in analiza signala, uporabnost pri študiju vezanja in strukturnih sprememb molekul. **Osnove metod sipanja** Uvod v statično in dinamično sipanje laserske svetlobe ter ozkokotno rentgensko sipanje, eksperimentalni sistemi, aplikacija, analiza in interpretacija rezultatov sipanja **Osmometrija** določanje molskih mas, osmoznih koeficientov in virialnih koeficientov z raznimi tipi osmometrov **Konduktometrične metode** Fizikalne osnove merjenja prevodnosti in transportnih števil v ionskih raztopinah, uporabnost pri določevanju stopnje vezave protiionov na polielektrolit. **Ionoselektivne elektrode** Fizikalne osnove, klasifikacija, priprava elektrod, uporabnost pri študijah koeficientov aktivnosti enostavnih elektrolitov in surfaktantov. **Eksperimentalne osnove merjenja fizikalnih lastnosti tekočin** (gostota, površinska napetost, viskoznost) **Difuzija topljenca v raztopinah** koeficient lastne difuzije, koeficient kemijske difuzije. Pomen koeficienta difuzije pri proučevanju transportnih in asociacijskih pojavov v raztopinah. Eksperimentalno določanje koeficientov difuzije.	study of (induced) asymmetry of the molecules. **Fluorimetry** Molecular basis of the signal, measurement and analysis of the signal, usefulness in the study of binding and structural changes of molecules. **Basics of scattering methods** Introduction to static and dynamic laser light scattering and small angle X-ray scattering, experimental systems, applications, data analysis and interpretation of the results. **Osmometry** Determination of molecular weights, osmotic coefficients and virial coefficients using various types of osmometers **Conductometric methods** Physical basics of conductivity and transference number measurements of ionic solutions, usefulness in determining the degree of binding of counterions to the polyelectrolyte. **Ion-selective electrodes** Physical basis, classification, preparation of electrodes, usefulness in studies of activity coefficients of simple electrolytes and surfactants. **Experimental basis of measuring physical properties of liquids** (density, surface tension, viscosity) **Diffusion of the solute in solution** Coefficient of self diffusion, coefficient of chemical diffusion. The importance of diffusion coefficient when considering transport and association phenomena in solution. Experimental determination of diffusion coefficients.

Temeljna literatura in viri / Readings:

- *Biocalorimetry, J.E Ladbury. in B.Z. Chowdhry, J. Wiley & Sons (1998), 345 str., (20 %).*
- *Principles of Physical Biochemistry, K.E. van Holde, Prentice Hall (1998), 657 str., (5 %).*
- *Biophysical Chemistry, A. Cooper, RSC, Cambridge (2004), 184 str., (10 %).*
- *Physical chemistry, W.J. Moore, Addison Wesley Longman (1996), 977 str. , (5 %).*
- *Small Angle X-ray Scattering, O. Glatter, O. Kratky, Academic Press (1982), 514 str., (25 %)*
- *Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter, P. Lindner in T. Zemb, Elsevier (2002), 541 str., (15 %).*
- *Polyelectrolytes, H. Dautzenberg, Hanser Publishers (1994), 343 str., (5%).*
- *Physical Methods of Chemistry: Electrochemical Methods, urednika B.W. Rossiter in J.F. Hamilton, J. Wiley & Sons (1986), 2. izdaja, 904 str.*
- *Experiments in Physical Chemistry, C. W. Garland, J. W. Nibler in D. P. Shoemaker, McGraw-Hill*

(2009), 8. izdaja, 734 str.

Dopolnilna literatura:

- Light Scattering Principles and Development, W. Brown,Claredon Press (1996), 528 str.

- Scattering in Polymeric and Colloidal Systems, W. Brown, K. Mortensen, Gordon and Breach Science Publishers (2000), 592 str.

- Light Scattering from Polymer Solutions and Nanoparticle Dispersions, Wolfgang Schaertl, Springer Verlag (2010), 205 str.

Cilji in kompetence:

Cilj predmeta je študentom predstaviti osnovne koncepte različnih eksperimentalnih metod in inštrumentov, ki se uporabljajo na področju fizikalne kemije, jih podrobneje seznaniti z eksperimentalnimi veščinami ter aplikacijami teh metod in jih spodbuditi, da pridobljeno znanje in izkušnje s pridom uporabljajo pri svojem bodočem delu.
Študentje pri predmetu pridobijo naslednje specifične *kompetence:*

- razumevanje teorijskega ozadja eksperimentalnih metod in inštrumentov,
- sposobnost presoje in pravilnega pristopa k uporabi različnih eksperimentalnih metod v fizikalni kemiji,
- sistematičnost pristopa pri reševanju projektne naloge,
- usposobljenost za samostojno delo na inštrumentih uporabljenih pri projektni nalogi in za izdelavo poročil.

Objectives and Competences:

The aim of the course is to introduce the basic concepts of different experimental methods and instrumentation used in the field of physical chemistry, to acquaint students with the experimental skills and applications of these methods and to encourage students to use this knowledge and experience in their future work.
Students of the course gain the following specific competencies:

- Understanding of theoretical background of experimental methods and instrumentation,
- Judgment and the proper approach to the use of different experimental methods in physical chemistry,
- A systematic approach in solving experimental problems
- Ability to work independently with the instruments in the labwork and to write reports.

Predvideni študijski rezultati:

Znanje in razumevanje

Osnovno teorijsko in praktično znanje ter razumevanje raznih eksperimentalnih tehnik v fizikalni kemiji: kalorimetrija, spektrometrija, statično in dinamično sipanje, osmometrija, površinska napetost, viskoznost, gostota, prevodnost, mikroskopija, …
Poznavanje osnov analize in interpretacije rezultatov meritev pri posamezni metodi.

Intended Learning Outcomes:

Knowledge and Comprehension

Theoretical and practical knowledge and understanding of various experimental techniques in physical chemistry: calorimetry, spectroscopy, static and dynamic scattering, osmometry, surface tension , viscosity, density, conductivity, microscopy. Knowing the basis of analysis and interpretation of measurement results for each method.

Uporaba Uporaba kalorimetričnih, spektrometričnih in osmometričnih metod, metod sipanja in drugih fizikalnih metod za določitev fizikalnih lastnosti raznih bioloških in koloidnih sistemov, raznih raztopin ter fizikalnih značilnosti kemijskih reakcij oziroma procesov.	Application Using calorimetric, spectroscopic, osmometric, scattering and other physical methods for determining the physical properties of various biological and colloidal systems, solutions and various physical properties of chemical reactions and processes.
Refleksija Študent bo pridobil občutek za povezavo med teorijskim ozadjem določene metode, inštrumentom in eksperimentalno izvedbo meritev. S pridobljenim znanjem bo kritično presodil in ovrednotil rezultate eksperimentalnih vaj in projektne vaje.	Analysis Students will gain a feeling for connection between the theoretical background of a particular method, instrument and experimental measurement. The knowledge gained will enable students to critically evaluate the results of experimental work.
Prenosljive spretnosti Sistematičnost pristopa pri reševanju projektne naloge, zbiranje literature, ovrednotenje in poročanje o rezultatih projekta.	Skill-transference Ability Systematic approach to solving the experimental problems, collecting of literature, evaluating and reporting on the results of the project.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, eksperimentalne praktične vaje, projektna vaja.	Lectures, seminars, laboratory exercises.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit po uspešno opravljenih vajah. Ocene: pozitivno (6-10), negativno (1-5).		Written examination after successful completion of laboratory exercises. Grades: (6-10) pass, (1-5) fail.

Reference nosilca / Lecturer's references:

LAH, Jurij, POHAR, Ciril, VESNAVER, Gorazd. Calorimetric study of the micellization of alkylpyridinium and alkyltrimethylammonium bromides in water. J. Phys. Chem., B Mater. surf. interfaces biophys., 2000, vol. 104, no. 11, str. 2522-2526.

LAH, Jurij, MAIER, Norbert M., LINDNER, Wolfgang, VESNAVER, Gorazd. Thermodynamics of binding of (R)- and (S)-dinitrobnzoyl leucine to cinchona alkaloids and their tert-butylcarbamate derivatives in methanol : evaluation of enantioselectivity by spectroscopic (CD, UV) and microcalorimetric (ITC) titrations. J. Phys. Chem., B Mater. surf. interfaces biophys., 2001, vol. 105, no. 8, str. 1670-1687.

DROBNAK, Igor, VESNAVER, Gorazd, LAH, Jurij. Model-based thermodynamic analysis of reversible unfolding processes. J. Phys. Chem., B Condens. mater. surf. interfaces biophys., 2010, vol. 114, no. 26, str. 8713-8722.

CERAR, Janez, ŠKERJANC, Jože: Electric transport and ion binding in solutions of fullerenehexamalonic acid Th-C66(COOH)12 and its alkali and calcium salts. J. Phys. Chem. B,

2008, 112, str. 892-895.
CERAR, Janez, URBIČ, Tomaž: Viscosity and electrophoretic mobility of cesium fullerenehexamalonate in aqueous solutions : comparing experiments and theories on nanometer-sized spherical polyelectrolyte. J. Phys. Chem. B, 2008, 112, str. 12240-12248.
ŠKERJANC, Jože, KOGEJ, Ksenija, CERAR, Janez: Equilibrium and transport properties of alkylpyridinium bromides. Langmuir, 1999, 15, str. 5023-5028.
TOMŠIČ, Matija, BEŠTER-ROGAČ, Marija, JAMNIK, Andrej, KUNZ, Werner, TOURAUD, Didier, BERGMANN, Alexander, GLATTER, Otto. Nonionic surfactant Brij 35 in water and in various simple alcohols : structural investigations by small-angle x-ray scattering and dynamic light scattering. J. phys. chem., B Condens. mater. surf. interfaces biophys., 2004, vol. 108, no. 22, str. 7021-7032
TOMŠIČ, Matija, JAMNIK, Andrej, FRITZ, Gerhard, GLATTER, Otto, VLČEK, Lukáš. Structural properties of pure simple alcohols from ethanol, propanol, butanol, pentanol, to hexanol : comparing Monte Carlo simulations with experimental SAXS data. J. phys. chem., B Condens. mater. surf. interfaces biophys., 2007, vol. 111, no. 7, str. 1738-1751.
TOMŠIČ, Matija, GLATTER, Otto. From bulk to dispersed hierarchically organized lipid phase systems. V: IGLIČ, Aleš (ur.). Advances in planar lipid bilayers and liposomes : volume 12, (Advances in planar lipid bilayers and liposomes). Amsterdam; Elsevier: Academic Press, cop. 2010, str. 167-200.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	ELEKTROKEMIJA
Course Title:	ELECTROCHEMISTRY

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: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
50	**25**	**/**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: prof. dr. Miran Gaberšček / Dr. Miran Gaberšček, Full Professor
Doc. dr. Janez Cerar / Dr. Janez Cerar, Assistant Professor

Jeziki / Languages:

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

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:

ELEKTROKEMIJA RAZTOPIN

Osnovni pojmi

Elektrokemija: raztopine elektrolitov, elektrodni procesi. Električni dvosloj. Voda kot najpomembnejše topilo. Vodikova vez. Sile v raztopinah. Solvatacija ionov. Hidrofobni efekt. Enostavni elektroliti. Polielektroliti. Ionske tekočine.

Termodinamične lastnosti raztopin elektrolitov

Različni nivoji opisa raztopin elektrolitov. Preprosti model raztopine elektrolita. Poisson-Boltzmannova enačba. Debye-Hücklova teorija. Srednji elektrostatski potencial. Prostorske porazdelitvene funkcije. Osmozni

Content (Syllabus outline):

ELECTROCHEMISTRY OF SOLUTIONS

Basic concepts

Electrochemistry: ionics and electrodics. Electric double-layer. Role of water as a solvent. Hydrogen bond. Forces in solutions. Solvatation of ions. Hydrophobic effect. Simple electrolytes. Polyelectrolytes. Ionic liquids.

Thermodynamic properties of electrolyte solutions

Different levels of electrolyte solution description. Simple model of electrolyte solution. Poisson-Boltzmann equation. Debye-Hückel theory. Mean electrostatic potential. Spatial distribution functions. Osmotic pressure and activity coefficient. Experimental

tlak in koeficient aktivnosti. Eksperimentalno določanje termodinamičnih količin. Pitzerjeva teorija. Asociacija ionov. Bjerrumova teorija.
Transportne lastnosti raztopin elektrolitov
Prevodnost. Difuzija elektrolitov.
Lastnosti raztopin polielektrolitov
Manningov model nabite premice. Hoffmeistrova vrsta. Osmozni koeficient. Razredčilne toplote. Membransko ravnotežje. Topnost polielektrolitov. Raba polielektrolitov. Biopolielektroliti.

ELEKTRODNI PROCESI
Pregled teorije elektrodnih procesov: Električni dvosloj ob elektrodah, kinetika elektrodnih procesov, Butler-Volmerjeva enačba in njene limitne oblike (Taflova relacija, polarizacijska upornost). Transport snovi (difuzija, konvekcija, migracija) in vpliv transporta na hitrost elektrodnih procesov.

Metode za študij elektrodnih procesov in ugotavljanje mehanizma elektrodnih procesov:
Potenciostatsko in galvanostatsko merjenje polarizacijskih krivulj, tranzientne tehnike (kronoamperometrija, kronokulometrija, kronopotenciometrija), ciklična voltametrija, impedančna spektroskopija. Simulacija elektrodnih procesov. Mehanizem izločanja vodika (HER) in redukcije kisika (ORR).

Elektrokemija materialov
- Elektrodepozicija, elektrosinteza in tehnike za študij procesov. Samosestavljive monoplasti-SAM, podnapetostno izločanje-UPD, elektrokemijska kvarčna mikrotehtnica-EQCMB.
- Elektrokemijska korozija: vrste korozije, termodinamski in kinetični vidiki (Pourbaix, Wagner-Traud), korozijski tok in korozijski potencial, Evansovi diagrami, elektrokemijske metode za študij korozijskih procesov, inhibicija korozije, pasivacija in protikorozijska zaščita.
- Elektrokemijski viri energije: elektrokemijski vidiki primarnih in sekundarnih virov energije (učinkovitost, gostota energije), pregled

determination of thermodynamic quantities. Pitzer theory. Ion association. Bjerrum theory.
Transport properties of electrolyte solutions
Conductivity. Diffusion of electrolytes.
Properties of polyelectrolyte solutions
Manning model. Hoffmeister series. Osmotic coefficient. Enthalpies of dilution. Membrane equilibrium. Solubility of polyelectrolytes. Application of polyelectrolytes. Biopolyelectrolytes.

ELECTRODE PROCESSES
Overview of the theory of electrode processes: electrical double layer at electrodes, kinetics of electrode processes, Butler-Volmer equation and the limiting cases (Tafel relation, polarisation resistance). Transport of matter(diffusion, convection, migration) and the influence on the rate of electrode processes. Methods for study of electrode processes and identification of their mechanisms: potentiostatic and galvanostatic measurements of polarisation curves, transient techniques (chronoamperometry, chronocoulometry, chronopotentiometry), cyclic voltammetry, impedance spectroscopy. Simulation of electrode processes. Mechanism of hydrogen (HER) and oxygen (OER) evolution reactions. Materials electrochemistry: electrodeposition, electrosynthesis and related phenomena. Self assembled monolayers (SAMs) underpotential deposition (UPD), electrochemical quartz crystal microbalance (EQCMB).
-Electrochemical corrosion: types of corrosion, thermodynamic and kinetic aspects (Pourbaix, Wagner-Traud), corrosion current and potential, Evans diagrams, electrochemical methods for investigation of corrosion, corrosion inbition, passivation and anticorrosion protection.
-Electrochemical energy sources (efficiency, energy density), overview of conventional and advanced systems (Zn/MnO_2, Pb/PbO_2, Ni/Cd, Ni/MH, Li/Li^+, fuel cells), photovoltaic systems.

klasičnih in naprednih sistemov (Zn/MnO_2, Pb/PbO_2, Ni/Cd, Ni/MH, Li/Li^+, gorivne celice), fotovoltaični sistemi.	

Temeljna literatura in viri / Readings:

Literatura (temeljna):

J. O'M. Bockris in A.K.N. Reddy *Modern Electrochemistry: ionics* (2. izdaja), New York: Plenum Press, 1998, 769 str. (cca 15 %).

J.O' M. Bockris, A.K.N. Reddy, *Modern Electrochemistry, Electrodics in Chemistry, Engineering, Biology, and Environmental Science*, Vol. 2B, 2nd Ed., Kluwer Academic/Plenum Publishers, New York, 2000.

M. Mandel *Physical Properties of Polyelectrolyte Solutions*, Pisa: Pacini Editore, 1999, 190 strani, (20 %).

Dodatna literatura:

M. R. Wright *An introduction to aqueous electrolyte solutions*, Chichester : J. Wiley, 2007, 574 str.

S. Forster in M. Schmidt, *Physical Properties of Polymers: Polyelectrolytes in Solution*, v Advances in Polymer Science, Berlin: Springer-Verlag, 1995.

A.J. Bard, M. Stratmann, Eds., *Encyclopedia of Electrochemistry*, Vol. 2, I*nterfacial Kinetics and Mass Transport*, Vol. Ed. E.J. Calvo, Wiley-VCH, Weinheim, 2003.

R. Greef, R. Peat, L.M. Peter, D. Pletcher, J. Robinson, *Instrumental Methods in Electrochemistry*, Ellis Horwood Lim., Chichester, 1985.

Cilji in kompetence:

Cilji:

Spoznavanje teorijskih pristopov pri obravnavi termodinamičnih in transportnih lastnosti raztopin elektrolitov in polielektrolitov.

Poglobljen študij elektrokemijskih zakonitosti, ki so podlaga za raziskave na področju elektroanaliznih tehnik, elektrokemije materialov, korozije in elektrokemijskih virov energije.

Kompetence:

Razumevanje fizikalnih pojavov v raztopinah elektrolitov in polielektrolitov ter elektrokemijskih procesov na elektrodah.

Uporaba tega znanja tako pri tehnoloških kot pri bioloških procesih.

Pridobljena znanja so usmerjena v razumevanje in usposabljanje za raziskovalno delo na teh področjih.

Objectives and Competences:

Objectives:

To get insight into basic theoretical approaches used in studies of thermodynamic and transport properties of both electrolyte and polyelectrolyte solutions.

In-depth study of electrochemical laws which represents the basis for understanding electroanalytical techniques, corrosion, materials electrochemistry and electrochemical energy sources.

Competences:

Understanding of physical phenomena occurring in electrolyte and polyelectrolyte solutions as well as electrochemical processes at electrodes. Application of this knowledge for comprehension of technological and biological processes.

Acquired knowledge is the basis for training and applied work either in research or in routine laboratory work in the field of electrochemistry.

Predvideni študijski rezultati:

Intended Learning Outcomes:

Znanje in razumevanje Študent pridobi temeljna znanja potrebna za razumevanje elektrokemijskih procesov in spozna uporabo elektrokemijskih zakonitosti na različnih področjih. Obvlada instrumentacijo in razume principe elektrokemijskih tehnik potrebnih za študij in raziskave povezanih z elektrokemijo.	Knowledge and Comprehension The student acquires base knowledge needed for understanding electrochemical processes and is acquainted with selected applications of electrochemical phenomena in various fields. The student also acquires selected laboratory skills and techniques related to electrochemistry.
Uporaba Pridobljeno znanje je usmerjeno v aplikacijo elektrokemijskih zakonitosti in pojavov na področjih kot so: korozija, preiskave in razvoj novih materialov, elektrokemijska sinteza in elektrokemijski viri energije, elektroanalizne metode, ipd. Študent se na teh področjih usposobi za samostojno raziskovalno delo in spozna načine prenosa in uporabe teoretskih zakonitosti v praksi.	Application Acquired base knowledge is implemented in selected applications such as: corrosion, investigation and development of new materials, electrochemical synthesis, electrochemical energy sources, electroanalytical methods etc. Student becomes qualified for independent research in the field and gets knowledge about transfer of theoretical concepts into practice.
Refleksija Pridobljeno teoretično znanje omogoča študentu poglobljen vpogled v osnovne koncepte in zakonitosti na področju elektrokemije. Dodatno študent pridobi veščine prenosa osnovnih znanj na izbrane praktične primere. Vsebina in izvedba predmeta predstavlja dobro osnovo za kasnejše aktivno in samostojno udejstvovanje na področju raziskav in uporabe elektrokemijskih znanj v praksi.	Analysis Acquired theoretical knowledge enables a profound insight into main concepts and laws in the field of electrochemistry. Additionally, the student acquires the ability to apply knowledge base into selected practical examples. The curriculum represents a solid background for later active and independent research in the fields of basic and applied electrochemistry.
Prenosljive spretnosti Pridobi veščine na področju elektrokemije, zna uporabljati znanstveno in strokovno literaturo ter pravilno predstaviti in razlagati merske rezultate. Pridobi znanja potrebna za projektno in timsko delo.	Skill-transference Ability Student acquires experimental skills in the field of electrochemistry, masters the use of scientific and professional literature and develops the skill of presenting and explaining complex and specific results to wider audience. Competences needed for project and team work are also developed.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji	Lectures, seminars

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit		Written exam

Reference nosilca / Lecturer's references:

1. **Janez Cerar**, Jože Škerjanc: Electric transport and ion binding in solutions of fullerenehexamalonic acid T_h-$C_{66}(COOH)_{12}$ and its alkali and calcium salts. *J. Phys. Chem. B,* 2008,

vol. 112, str. 892-895.
2. **Janez Cerar**, Jože Škerjanc: Water-soluble fullerenes. 3. Alkali salts of fullerenehexamalonic acid T_h-C_{66} $(COOH)_{12}$. *J. Phys. Chem. B,* 2003, vol. 107, str. 8255-8259.
3. **Janez Cerar**, Jože Škerjanc: Water-soluble fullerenes. 2. Sodium fullerenexamalonate T_h-C_{66} $(COONa)_{12}$, a highly asymmetric electrolyte. *J. Phys. Chem. B,* 2000, vol. 104, str. 727-730.

1. HODNIK, Nejc, ZORKO, Milena, JOZINOVIĆ, Barbara, BELE, Marjan, DRAŽIĆ, Goran, HOČEVAR, Stanko, **GABERŠČEK, Miran**. Severe accelerated degradation of PEMFC platinum catalyst : a thin film IL-SEM study. *Electrochem. commun.*, 2013, vol. 30, str. 75-78
2. KHATIB, R., DALVERNY, A. - L., SAUBANÈRE, M., **GABERŠČEK, Miran**, DOUBLET, M. - L. Origin of the voltage hysteresis in the CoP conversion material for Li-ion batteries. *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2013, vol. 117, no. 2, str. 837-849.
3. ATEBAMBA, Jean-Marcel, MOŠKON, Jože, PEJOVNIK, Stane, **GABERŠČEK, Miran**. On the interpretation of measured impedance spectra of insertion cathodes for lithium-ion batteries. *J. Electrochem. Soc.*, 2010, vol. 157, no. 11, str. A1218-A1228
4. DREYER, Wolfgang, JAMNIK, Janko, GUHLKE, Clemens, HUTH, Robert, MOŠKON, Jože, **GABERŠČEK, Miran**. The thermodynamic origin of hysteresis in insertion batteries. *Nature materials*, 2010, vol. 9, str. 448-453,
5. STRMČNIK, Dušan, **GABERŠČEK, Miran**, PIHLAR, Boris, KOČAR, Drago, JAMNIK, Janko. Copper dissolution in ammonia solutions : identification of the mechanism at low overpotentials. *J. Electrochem. Soc.*, 2009, vol. 156, no. 7, str. C222-C229.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	FIZIKALNA KEMIJA II
Course Title:	PHYSICAL CHEMISTRY II

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, 2nd Cycle	/	1st	2nd

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE214

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

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee / Dr. Barbara Hribar Lee, Full Professor

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

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:

Osnove: Merjenje, časovna odvisnost in časovno povprečje. Zakona statistične termodinamike. Opis mikroskopskega stanja. Kanonična porazdelitev. Povprečja in kolebanja okoli povprečne vrednosti, povezava s termodinamiko. Izolirani sistem. Odprt sistem, kolebanja koncentracije, stisljivost in stabilnost sistema. Drugi (N,p,T) sistemi.
Mrežni modeli: Flory-Hugginsova teorija.
Neodvisni podsistemi: Einsteinov model kristala. Paramagnetna snov. Fermi-Diracova in Bose–Einsteinova statistika. Boltzmannova statistika: razredčeni plini. Izračun konstante kemijskega ravnotežja. Adsorbcija, Langmuirjeva in B.E.T. izoterma, vezanje ligandov na makromolekulo.

Content (Syllabus outline):

Introduction: Time-average of measured quantity. Laws of statistical thermodynamics. Description of microscopic state of a system. Canonical distribution. Averages and fluctuations; the relations with thermodynamics. Isolated system. Open system, concentration fluctuations, compressibility, stability of the system. Other (N,p,T) systems.
Lattice models: Flory-Huggins theory
Independent subsystems: Einstein model of crystal. Paramagnetic materials. Fermi-Dirac and Bose-Einstein statistics. Boltzmann statistics: diluted gasses. Evaluation of the chemical equilibrium constant. Adsorption,

Klasična statistična termodinamika: Konfiguracijski integral in povprečja. Parski potencial. Računalniške simulacije, metoda Monte Carlo, molekulska dinamika. Teorije na osnovi parske porazdelitvene funkcije. Računanje termodinamičnih količin (notranja energija, enačbe stanja). Osnove termodinamične perturbacijske teorije.	Langmuir and B.E.T. isotherms, ligand binding to macromolecules. Classical statistical thermodynamics: Configuration integral and averages. Pair potential. Introduction to computer simulations, Monte Carlo method, molecular dynamics. Evaluation of thermodynamic quantities (internal energy, equation of state). An introduction to thermodynamic perturbation theory.

Temeljna literatura in viri / Readings:

- Friedman, H. L., *A Course in Statistical Mechanics*, New Jersey: Prantice-Hall, 1985, pp 1-109.
- Hill, T. L., *Introduction to Statistical Thermodynamics*, Reading: Addison-Wesley, 1960, pp 124-188.
- V. Vlachy, B. Hribar Lee: Fizikalna kemija II - Uvod v statistično termodinamiko, skripta

Dodatna literatura:
- K. A. Dill, S. Bromberg, Molecular Driving Forces, Garland Science, 2011.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Naloga statistične termodinamike je, da iz podatkov o lastnostih atomov in molekul ter sil med njimi izpelje makroskopske lastnosti snovi. Na ta način omogoča molekularno interpretacijo merskih podatkov. *Kompetence:* V prvem delu obravnavamo osnove statistične termodinamike, le−te omogočajo globje razumevanje pojavov kot so toplota, entropija, termodinamično povprečje, kolebanje okoli povprečne vrednosti in drugi. Drugi del predmeta je namenjen prikazu posameznih primerov uporabe statistične termodinamike v kemiji in sorodnih vedah.	***Objectives:*** The purpose of statistical thermodynamics is to predict macroscopic properties of a given thermodynamic system, using as input the knowledge about constituent atoms (or molecules) and intermolecular forces between them. It makes possible to interpret the experimental data from molecular point of view. ***Competences:*** Profound understanding of thermodynamic quantities, such as heat, entropy, thermodynamic averages, fluctuations, and others. Application to real chemical and physical problems.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Poznavanje osnov statistične termodinamike, ki jih obravnava predmet Fizikalna kemija, omogoča globlje razumevanje pojmov iz fizikalne kemije ter interpretacijo eksperimentalnih podatkov na osnovi lastnosti atomov in molekul.	Knowledge and Comprehension The basic knowledge of statistical thermodynamics that is the subject of this course enables the students a deeper understanding of the physical chemistry concepts, as well as the interpretations of the experimental data in view of the properties of atoms and molecules.
Uporaba Pri tem predmetu se spoznamo z modernimi	Application The students get to know the modern

teoretičnimi metodami za študij lastnosti snovi. Metode se uporabljajo v kemiji, farmaciji in biologiji, pa tudi pri načrtovanju različnih tehnoloških procesov kot so, na primer, separacijske metode. Predmet je osnova raziskovalnemu delu na področju kemije.	theoretical methods used for studying the properties of different substences. The methods are used in chemistry, pharmacy and biology, as well as in planning different technologocal processes, such as separation methods. The course is prociding the bases for the research work in the chemistry field.
Refleksija Znanja, ki jih študent osvoji pri tem predmetu, pomagajo pri kritičnem vrednotenju merskih podatkov, razumevanju lastnosti fizikalnih sistemov in s tem omogočajo kvalitetno in samostojno delo na drugih področjih kemije.	Analysis The knowledge that the students obtain via this course is meant to be used in the critical assesment of measuring data, as well as the understanding the system properties which is neede in different areas of chemistry.
Prenosljive spretnosti Spretnosti uporabe domače in tuje literature in drugih virov, identifikacija in reševanje problemov, kritična analiza rezultatov, kvantitativno razumevanje drugih (bolj opisnih) predmetov.	Skill-transference Ability The ability of using different literature, as well as other resources, identification and problem solving, critical evaluation of the results, quantitative interpretation of knowledge obtained in other courses.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja, seminarji.	- Lectures - Seminars

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni (nadomestita ga lahko dva pozitivno ocenjena kolokvija) in ustni izpit.		Written and oral exam.

Reference nosilca / Lecturer's references:

1. MOHORIČ, Tomaž, HRIBAR-LEE, Barbara, VLACHY, Vojko. Effects of the translational and rotational degrees of freedom on the hydration of simple solutes. The Journal of chemical physics, ISSN 0021-9606, 2014, vol. 140, no. 18, art. no. 184510 (str. 1-7).
2. MOHORIČ, Tomaž, URBIČ, Tomaž, HRIBAR-LEE, Barbara. The application of the integral equation theory to study the hydrophobic interaction. The Journal of chemical physics, ISSN 0021-9606, 2014, vol. 140, no. 2, art. no. 024502 (6 str.).
3. HRIBAR-LEE, Barbara, LUKŠIČ, Miha, VLACHY, Vojko. Partly-quenched systems containing charges. Structure and dynamics of ions in nanoporous materials. Annual reports on the progress of chemistry. Sectin C, Physical chemistry, ISSN 0260-1826, 2011, vol. 107, no. 1, str. 14-46.

UČNI NAČRT PREDMETA/COURSE SYLLABUS	
Predmet:	FOTOKEMIJA IN RADIKALI
Course Title:	PHOTOCHEMISTRY AND RADICALS

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: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	15	LV 15	/	/	75	5

Nosilec predmeta / Lecturer: Izr. prof. dr. Jernej Iskra / Dr. Jernej Iskra, Associate 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):**
Organska fotokemija. a) Uvod. Interakcija spojin z elektromagnetnim valovanjem, delovanje mikrovalov in ultrazvoka. Absorpcija svetlobe, elektronska stanja in prehodi, lastnosti vzbujenih stanj, Jablonskijev diagram, kvantni izkoristek, prenos energije, dušenje. b) Fotokemične reakcije. Izomerizacije, fragmentacije, adicije, substitucije, eliminacije, premestitve, , periciklične reakcije. c) Foto elektron transfer, fotokataliza, kemiluminiscenca, singletni kisik, fotokemija v okolju. **Kemija radikalov.** a) Uvod. Lastnosti radikalov. Reaktivnost in stabilnost radikalov, delokalizacija in	**Organic photochemistry** a) Introduction: Interaction of compounds and electromagnetic radiation mode of action of microwaves and ultrasound. Absorption of light, electronic states and transitions, properties of excited states, Jablonski diagram, quantum yield, energy transfer, quenching. b) Photochemical reactions: isomerizations, fragmentation, additions, substitutions, eliminations, rearrangements, pericyclic reactions c) Photo electron transfer, photocatalysis, kemiluminescence, singlet oxygen, environmental photochemistry. **Chemistry of radicals** a) Introduction: Properties of radicals, reactivity

elektronski efekti. Metode za tvorbo radikalov. b) Metode za detekcijo in opazovanje radikalov in vzbujenih stanj (ESR, laserska bliskovna fotoliza) c) Reakcije radikalov, značilnosti radikalskih reakcij, verižne reakcije, inhibicija. d) Pomembne radikalske reakcije v organski sintezi. **Polimeri** a) Uvod. Naravni polimeri, vrste polimerov, fizikalne lastni polimerov. b) Polimerizacija, vrste polimerizacije, reakcije na polimerih (zamreženje, graft polimerizacija), pretvorbe funkcionalnih skupin. c) Recikliranje, novi polimerni materiali.	and stability, delocalization and electronic effects, formation of radicals. b) Methods for detection and observation of radicals (ESR, Laser flash photolysis). c) Radical reactions: characteristics of radical processes, chain reactions, inhibition. d) Radical reactions in organic synthesis. **Polymers** a) Introduction. Natural polymers, types of polymers, physical properties of polymers. b) Polymerization, types of polymerization, reactions on polymers (crosslinking, graft polymerization), transformation of functional groups. c) Recycling, novel polymeric materials.

Temeljna literatura in viri / Readings:

- *Modern Physical Organic Chemistry*, Eric V. Anslyn e tal., University Science Books, 2006 (izbrana poglavja).

Dodatna literatura:

- *Principles and Applications of Photochemistry*, Brian Wardle, Wiley, 2009.
- *Advanced Free Radical Reactions for Organic Synthesis*, Hideo Togo, Elsevier, 2004.
- *Principles of Polymer Chemistry*, Third Edition, A. Ravve, Springer, 2012.

Cilji in kompetence:	**Objectives and Competences:**
Cilji predmeta Študent nadgradi znanja iz področij fotokemije in kemije radikalov in polimerov. Predmet seznani študente s spremembami organskih molekul pod vplivom svetlobe v plinasti fazi, raztopinah, v prisotnosti vzbujevalcev in v heterogenih sistemih ter s procesi v okolju. Študent spozna osnovne značilnosti in uporabo radikalskih reakcij in se nauči izvajati omenjene pretvorbe v laboratoriju. Spozna osnovne reakcije priprave in modifikacij polimerov ter osnove o lastnostih polimerov.	Learning outcomes Student acquires a new knowledge about the photochemical and photophysical phenomena and reactions. A student gets insight into the transformations of organic molecules under the influence of light and in the presence of sensitizers. Basic understanding of radicals and their reactions is supplemented by more detailed expertise about the properties of radicals, their behavior, typical radical reactions and synthetic use. Synthesis and properties of polymers, modification of polymer structure and functionality.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Poznavanje narave in uporabe fotokemičnih procesov ter pomen fotokemičnih reakcij v okolju. Lastnosti radikalov. Značilnosti radikalskih procesov, uporaba radikalskih reakcij v sintezi.	Knowledge and Comprehension Characteristics of photochemical processes, their uses and importance of photochemical reactions in the environment. Properties of radicals. Characteristics of radical reactions, use in synthesis. Undesired radical

Neželjeni procesi in preprečevanje. Osnovne lastnosti in reakcije pridobivanja polimerov, modifikacije in uporaba polimerov v kemiji.	processes and their inhibition. Basics of syntheses of polymers, modification and uses of polymers in chemistry.
Uporaba Študent bo znal izbrati, zasnovati in uporabiti fotokemične in radikalske reakcije za sintezo organskih spojin in polimerov. Poznavanje neželenih radikalskih reakcij in njihovo preprečevanje. Poznavanje načinov priprave različnih polimernih materialov in njihovih lastnosti ter transformacij.	Application Ability to choose, to design and to apply photochemical or radical reactions for the synthesis of organic materials or polymers. Knowledge about photochemical or oxidative deterioration reactions of organic materials and their inhibition. Preparation and modification of polymeric materials to attain desired properties or functionality.
Refleksija Študent bo znal ugotoviti, kdaj poteka kemijski proces po fotokemični poti in kdaj je neka reakcija radikalska oziroma ionska. Z uporabo znanj, dobljenih pri tem predmetu bo znal voditi proces v želeno smer.	Analysis Student will be able to distinguish photochemical and thermal processes, as well as radical and ionic ones.
Prenosljive spretnosti -Dostopanje do literaturnih virov -Zbiranje, interpretacija in kritično vrednotenje podatkov -Identifikacija in reševanje problemov	Skill-transference Ability Access to literature sources. Collection, interpretation and critical assessment of scientific information. Problem identification and solving.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji, laboratorijske vaje	Lectures, seminar, laboratory work

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit Ustni izpit Pogoj za pristop k izpitu je uspešno opravljeno praktično delo		Written exam Oral exam Accomplished practical work is a prerequisite to exam attendance.

Reference nosilca / Lecturer's references:

- KAWADA, Kosuke, OKANO, Koji, **ISKRA, Jernej**, KRAJNC, Peter, CAHARD, Dominique. Selectfluor[sup](TM) on a PolyHIPE material as regenerative and reusable polymer-supported electrophilic fluorinating agent. *Advanced Synthesis & Catalysis*, ISSN 1615-4150. [Print ed.], 2017, vol. 359, no. 4, str. 584-589, doi: 10.1002/adsc.201601312. [COBISS.SI-ID 30090791]
- MOŽINA, Štefan, STAVBER, Stojan, **ISKRA, Jernej**. Dual catalysis for the aerobic oxidation of benzyl alcohols - nitric acid and fluorinated alcohol. *European journal of organic chemistry*, ISSN 1434-193X, 2017, vol. 2017, no. 3, str. 448-452, doi: 10.1002/ejoc.201601339. [COBISS.SI-ID 30184487]

- BEDRAČ, Leon, **ISKRA, Jernej**. Iodine(I) reagents in hydrochloric acid-catalyzed oxidative iodination of aromatic compounds by hydrogen peroxide and iodine. *Advanced Synthesis & Catalysis*, ISSN 1615-4150. [Print ed.], 2013, vol. 355, no. 7, str. 1243-1248, doi: 10.1002/adsc.201300127. [COBISS.SI-ID 26709799]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	KARAKTERIZACIJA IN STABILNOST MATERIALOV KULTURNE DEDIŠČINE
Course Title:	CHARACTERISATION AND STABILITY OF MATERIALS FROM CULTURAL HERITAGE

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	/	2.	4.
USP Chemistry, 2nd Cycle	/	2nd	4th

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I15

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

Nosilec predmeta / Lecturer: doc. dr. Irena Kralj Cigić / Dr. Irena Kralj Cigić, Assistant Professor

Jeziki / Languages:

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

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:

Materiali kulturne dediščine – uvod.
Osnove študija materialov kulturne dediščine– razumevanje kompleksnosti nehomogene in nedoločene sestave naravnih in naravno staranih materialov, starosti (metode datiranja) in provenience (arheometrija).
Stabilnost materialov kulturne dediščine.
Termoliza. Termooksidacija. Procesi razgradnje materialov pod vplivom kisika, avtooksidacija, antioksidanti. Fotoliza in fotooksidacija. Razgradnja pod vplivom onesnaževal. Vpliv SO_2, ozona, NO_x.
Metode stabilizacije materialov kulturne dediščine.
Metode za študij trajnosti materialov kulturne dediščine.

Content (Syllabus outline):

Cultural heritage materials – introduction.
Fundamentals of cultural heritage material studies – understanding of the complexity of inhomogeneous composition of natural and naturally aged materials, age (methods of dating) and provenience (archaeometry).
Stability of cultural heritage materials.
Thermolysis. Thermoxidation. Degradation processes of materials influenced by oxygen, autoxidation, antioxidants. Photolysis and photodegradation. The influence of pollutants. Influence of SO_2, ozone, NO_x.
Methods of stabilisation of cultural heritage materials.
Studies of durability of cultural heritage materials.

Pospešena razgradnja, modelni eksperimenti in eksperimenti v realnem okolju. Analitika in karakterizacija razgradnih produktov, kinetika razgradnje, modeliranje, kontrolirana razgradnja. Modeliranje življenjske dobe. <u>Metode za karakterizacijo materialov kulturne dediščine.</u> Porušne in neporušne metode, definicija. Mikrovzorčevanje, prostorska resolucija in specifičnost. Prenosna instrumentacija. Kolorimetrija, rentgenske metode, spektroskopija infrardeče svetlobe, metode na osnovi laserjev, kromatografske metode. Lasersko oslikovanje (skeniranje) predmetov, stavb, prostorov in izdelava 3D modelov. <u>Monitoring okoljskih parametrov</u> Senzorji za svetlobo, indikatorji (dozimetri) in analizne metode za spremljanje kemijskih onesnaževal.	Methods of accelerated ageing, model experiments and experiments in real environment. Analytical methods and characterisation of degradation products, kinetics of degradation, modelling, controlled degradation. Modelling of lifetime. <u>Methods for cultural heritage material characterisation.</u> Destructive and non-destructive methods – definitions. Microsampling, spatial resolution and specificity. Portable instrumentation. Colourimetry, X-ray methods, IR spectroscopy, laser-based analytical methods, chromatographic methods. Laser scanning of objects, buildings and spaces and 3D imaging. <u>Monitoring of environmental parameters.</u> Light sensors, indicators (dosimeters) and analytical methods for analysis of indoor and outdoor pollutants.

Temeljna literatura in viri / Readings:

- M. Schreiner, M. Strlič: Handbook on the use of lasers in conservation and conservation science, COST, 2006. (elektronski vir)
- E. Ciliberto, G. Spoto, Modern analytical methods in art and archaeology. New York: John Wiley & Sons, 2000, 755 str. (25 %)

Dodatna literatura:

- Norman S. Allen, M. Edge, Fundamentals of Polymer Degradation and Stabilisation, Springer, 2001.
- Članki iz znanstvenih in strokovnih revij.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Študent se pri predmetu usposobi za raziskovalno delo na področju študija materialov kulturne dediščine, z upoštevanjem konteksta uporabe materiala in naravnih razgradnih procesov. *Kompetence:* Obravnava in uporaba specifičnih metod vzorčenja, analiznih metod in metod študija trajnosti materialov je povezana z obravnavano problematiko (case-studies) in nadgrajuje študentova predhodna znanja.	**Learning outcomes:** To gain knowledge of cultural heritage materials and fundamental analytical techniques in use for their characterisation. The student gains knowledge of environmental parameters affecting the lifetime expectancy of heritage materials and about the typical degradation processes. **Competences:** The course builds on case-studies and will provide an overview of sampling techniques, analytical methods and durability studies and thus builds on previous knowledge of chemistry

	and material science.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Študent bo razumel osnovne zakonitosti materialov kolturne dediščine - pojem trajnosti, razgradnje, življenjske dobe, zakonitosti razgradnih procesov in proceseter postopke razvoja procesov stabilizacije. Poznal bo osnovne postopke karakterizacije in evaluacije analiznih rezultatov.	Knowledge and Comprehension To gain understanding of basic principles of cultural heritage materials- terms of durability, degradation, lifetime, principles of degradation processes and procedures for development of conservation procedures.
Uporaba Študent bo znal uporabiti principe oz. zakonitosti na primerih, ter znal poiskati povezave s prakso. Znal bo utemeljiti razvoj novih postopkov stabilizacije.	Application To gain application of principle on real cases and to find connections with practical use. To validate development of new conservation procedures.
Refleksija Znal bo kritično ovrednotiti skladnosti med prakso in teorijo, neskladnosti bo znal evaluirati.	Analysis To critically evaluate consistency between theory and practice and to evaluate differences
Prenosljive spretnosti - sintetično, analitično, ustvarjalno mišljenje in reševanje problemov analitike in karakterizacije kulturne dediščine - uporaba znanja v praksi - iniciativnost/ ambicioznost, - osebna odgovornost in odgovornost do skupine, - vrednota stalnega osebnega strokovnega napredovanja	Skill-transference Ability - synthetic, analytical, creative thinking and solving analytical problems and characterisation of cultural heritage -application of knowledge in practice -initiative / ambition -personal responsibility and group responsibility -values of permanent personal and professional progression

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, ki vključujejo strokovne ekskurzije v raziskovalne inštitucije. Seminar: skupinsko in individualno projektno delo na izbrano tematiko, pisanje seminarske naloge, ustna predstavitev.	Lectures including visits of research institutions. Seminar: team and individual project work on selected theme, writing of seminar, oral presentation.

Delež (v %) /

Načini ocenjevanja:	Weight (in %)	**Assessment:**
Seminar	**40%**	Seminar
Pisni izpit	**60%**	Written exam
Ocenjevanje: 6-10 (pozitivno), 1-5 (negativno)		Grading scale: 6-10 (pozitive), 1-5 (negative)

Reference nosilca / Lecturer's references:

- M. Strlič, I. Kralj Cigić, J. Kolar, G. De Bruin, B. Pihlar. Non-destructive evaluation of historical paper based on pH estimation from VOC emissions. Sensors, 7 (2007) 3136-3145.
- M. Strlič, J. Thomas, T. Trafela, L. Csefalvayova, I. Kralj Cigić, J. Kolar, M. Cassar. Material degradomics : on the smell of old books. Analytical chemistry, 81 (2009) 8617-8622.
- K. L. Rasmussen, J. Gunneweg, J. Van Der Plicht, I. Kralj Cigić, A. D. Bond, B. Svensmark, M. Balla, M. Strlič, G. L. Doudna. On the age and content of Jar-35: a sealed and intact storage jar found on the southern plateu of Qumran. Archaeometry, 53 (2011) 791-808.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	KEMOMETRIJA
Course Title:	CHEMOMETRICS

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, 2nd Cycle	/	1st	2nd

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I11

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	15	15 SV	/	/	75	5

Nosilec predmeta / Lecturer: prof. dr. Matevž Pompe / Dr. Matevž Pompe, Full 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):
Definicija merskega prostora (skalarji, vektorji, razdalje) Predstavili bomo definicije merskega prostora ter opisov populacije ter vzorca. **Osnove napovedne statistike** Študenti se bodo spoznali z osnovnimi porazdelitvami, ki jih srečamo pri statističnih testih. Prav tako bodo dobili vpogled v predpostavke na katerih temeljijo obravnavani test. Detekcija izvenležečih točk. **Kalibracijska premica**, meja zaznavnosti Obravnavali bomo kalibracijsko premico na	**Definition of the measurement space** (scalar , vector , distance) We will present the definition of the measurement area and descriptions of the population and the sample. **Basics of predictive statistics** Students will learn the basic distributions encountered in statistical tests. They will also get an insight into the assumptions underlying the present test. Detection of outliers. **The calibration line** , the limit of detection The procedure to obtain calibration line will be explained in the case of equal or unequal

primeru enakih ali neenakih varianc v merskem prostoru. Poudarek bo na kasnejšem testiranju modela ter izračunu merske negotovosti ob upoštevanju enačbe premice.	variances in metric space. The focus will be on model validation and measurement uncertainty calculation taking into account the calibration line equation.
Izdelava modelov (linearni, nelinearni) V okviru tega poglavja bodo študenti spoznali osnove večkratne linearne regresije, PLS, PCR kot primeri linearne regresije, med nelinearnimi tehnikami pa bomo predstavili različne umetne nevronske mreže.	**Modeling** (linear and nonlinear) In this chapter, students will learn the basics of multiple linear regression , PLS, PCR as examples of the linear regression. As example of the non-linear techniques various artificial neural networks will be presented.
Transformacije merskega prostora Predstavili bomo nekatere pogoste transformacije merskega prostora (npr. PCA,...), ki jih uporabljamo za boljšo predstavitev več dimenzionalnih merskih prostorov.	**Transformation of the measurement space** Some common measurement space transformation will be presented (eg PCA , ...), which are used to enable the graphical presentation of the multi-dimensional metric spaces . 6 Filtering of noise Students will learn simple procedures for noise filtrations in the experimental measurements.
Optimizacija (genetski algoritem) ter eksperimentalni načrt Študenti bodo spoznali oba navedena postopka optimizacije v večdimenzionalnem merskem sistemu, kot tudi postopke večnivojskega načrtovanja eksperimentov z namenov zmanjšanja potrebnega števila meritev.	**Optimization** (genetic algorithm) and experimental design Students will learn about both procedures for optimization in multi-dimensional measurement system. They will gain knowledge on multi-level experimental design in order to reduce the number of required experiments.
Grupiranje Predstavili bomo enostavne postopke grupiranja podatkov v večdimenzionalnem merskem prostoru, kot tudi uporabo umetnih nevronskih mrež v te namene.	**Clustering** We will present a simple procedure for clustering of data in a multidimensional space of measurements, as well as the use of artificial neural networks for the same purpose.
Vrednotenje modelov Spoznali bomo osnovne postopke za delitev podatkov v več setov potrebnih za učenje in testiranje modela. Prav tako bomo obravnavali metode, ki jih uporabljamo pri testiranju različnih modelov.	**Model validation** We will learn the basic procedures for dividing data in different sets needed for model validation (learning and testing set). We will also discuss the methods used in various model validation.
Matematične reprezentacije kemijskih struktur Spoznali bomo nekatere enostavne reprezentacije kemijskih struktur, ki jih lahko uporabljamo pri modeliranju povezav med	**Mathematical representation of chemical structures** Some simple representations of chemical structures that can be used in modeling the

kemijsko strukturo in lastnostmi molekul (QSAR, QSPR). Osnove topoloških indeksov- **Razlike med različnimi tipi QSAR modelov** Modeli za odkrivanje novih zdravil, modeli za regulativo	relationship between chemical structure and properties of molecules (QSAR , QSPR) will be discussed. Basic concepts of topological indices. **Differences between various types of QSAR models.** Models used for drug discovery, models for regulatory purposes

Temeljna literatura in viri / Readings:

- D.L. Massart, B.G.M. Vandeginste, L.C.C. Buydens, S. De Yong, P.J.Lewi, J. Smeyers-Verbeke: handbook of Chemometrics and Qualimetrics, Elsevier, 2003 (700 strani, 30%).

Dodatno
ZUPAN, Jure. Kemometrija in obdelava eksperimentalnih podatkov. Ljubljana: Kemijski inštitut: Inštitut Nove revije, Zavod za humanistiko, 2009. 368 str., ilustr. ISBN 978-961-92463-3-7.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: a) Seznaniti študente s teorijo in uporabo kemomentričnih metod za: • Pripravo eksperimentov • Predobdelavo merskih podatkov • Vrednotenje podatkov in rezultatov dobljenih pri eksperimentih z večjim številom spremenljivk b) Podati osnove modeliranja, iskanja inverznih modelov ter vrednotenja statistične zanesljivosti dobljenih modelov. c) Omogočiti študentom neposredni dostop do računalnikov ter ustrezne programske opreme za izvedbo naštetih testov. *Kompetence:* Študent bo usposobljen kritično ovrednotiti eksperimentalne podatke, poiskati vzorce v večdimenzionalnih merskih prostorih ter izdelati nekatere enostavne modele, ki povezujejo merski prostor z določeno lastnostjo opazovanega sistema.	**Objectives** a) To acquaint students with the theory and applications of chemometric procedures for: • Preparation of experiments • Pretreatment of experimental data • Evaluation of data and results obtained from experiments with a large number of variables b) Provide the basics of modeling, search for inverse models and the statistical evaluation of the obtained models. c) To allow students direct access to computers and relevant software for carrying out the above tests. **Competences** Student will be able to critically evaluate experimental data to find patterns in multi-dimensional metric spaces, and create some simple models to use measurement space in order to explain some characteristics of the observed system.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Študent se bo naučil kritično uporabljati kemometrične metode. Razumeti bo moral njihovo delovanje. Pri predmetu bo spoznal njihove bistvene prednosti ter omejitve.	<u>Knowledge and Comprehension</u> The students will learn to critically apply chemometric methods. They will understand their operation as well as their main advantages and limitations.

Uporaba Znanja bodo uporabljena v analiznih laboratorijih za zagotavljanje kakovosti rezultatov. Prav tako se bodo znanja uporabljala pri raziskavah v okolju ter analizi živil za razpoznavanje vzorcev ter izdelavi napovednih modelov.	Application Knowledge will be used in analytical laboratories to ensure the quality of the results. The obtained knowledge will be used in the environmental and food research for pattern recognition and the creation of predictive models.
Refleksija Študent bo sposoben samostojno obdelovati eksperimentalne podatke v večdimenzionalnem vektorskem prostoru, v njih poiskati skrite vzorce ter izdelati in validirati enostavne linearne modele.	Analysis Students will be able to independently process the experimental data in multi-dimensional vector space and find the hidden patterns and to establish and validate a simple linear models.
Prenosljive spretnosti Študenti se naučijo kritično podajati in interpretirati eksperimentalne rezultate in izdelati ter validirati enostavne modele.	Skill-transference Ability Students learn to critically present and interpret experimental results and to create and validate simple models.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja s seminarji.	Lectures and seminar work.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni in ustni izpit. ocene od 6-10 (pozitivno) oz. 1-5 (negativno).		Written and oral exam Grades: positive 6-10; negative 1-5.

Reference nosilca / Lecturer's references:

1. **POMPE, Matevž**, DAVIS, Joe M., SAMUEL, Clint D. Prediction of thermodinamic parameters in gas chromatography from molecular structure : hydrocarbons. *J. chem. inf. comput. sci.*, 2004, vol. 44, no. 2, str. 399-409.
2. **POMPE, Matevž**. Variable connectivity index as a tool for solving the 'anti-connectivity' problem. *Chem. Phys. Lett.*. [Print ed.], 2005, vol. 404, no. 4/6, str. 296-299.
3. KOLAR, Jana, ŠTOLFA, Andrej, STRLIČ, Matija, **POMPE, Matevž**, PIHLAR, Boris, BUDNAR, Miloš, SIMČIČ, Jurij, REISSLAND, Birgit. Historical iron gall ink containing documents - properties affecting their condition. *Anal. chim. acta*. [Print ed.], 2006, vol. 555, str. 167-174.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	KOORDINACIJSKA KEMIJA
Course Title:	COORDINATION CHEMISTRY

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

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I01

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
15	15	45 LV	/	/	75	5

Nosilec predmeta / Lecturer: doc. dr. Bojan Kozlevčar / Dr. Bojan Kozlevčar, 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):
Vsebina predmeta Koordinacijska kemija predstavlja nadaljevanje in nadgradnjo vsebine predmetov s področja anorganske kemije z dodiplomske stopnje (predmet Anorganska kemija II). Natančna karakterizacija spojin temelji na povezavi podatkov iz strukturne analize in analize realnega vzorca s povdarkom na: - določanju čistosti in istovetnosti snovi z znano spojino - ugotavljanju vrste kemijskih vezi v spojini - določanju načina koordinacije ligandov - opisu koordinativne sfere kovinskega iona - primerjavi strukturnih in analiznih podatkov s podatki kemijsko sorodnih spojin Splošne vsebine bodo predelali na predavanjih in seminarjih, praktične na vajah v laboratoriju.	A content of the subject Coordination Chemistry represents a continuation and upgrade of other subject contents in the inorganic chemistry field of the first cycle study programs (subject Inorganic Chemistry II) . The precise characterization of compounds is based on data correlation from the structural analysis and real samples analysis focussing on: - Purity and identity determination of the known compound - A type of the chemical bond analysis within the compound - Determining the ligands coordination mode - The coordination sphere of the metal ion description - A comparison of structural and analytical data with chemically related compounds

Vsebina vaj: Sinteza koordinacijaskih spojin na osnovi znanih literaturnih podatkov. Temu sledi natančna karakterizacija spojin s spektroskopskimi metodami, merjenjem magnetnih lastnosti ter prevodnosti. Vaje obsegajo uporabo metod rentgenske praškovne difrakcije, infra-rdeče in UV-vidne spektroskopije, magnetne susceptibilnosti ter električne prevodnosti. Dodatno se študentom predstavita tudi metodi elektronske paramagnetne in nuklearne magnetne resonance (EPR, NMR). Metode karakterizacije ter primeri spojin so izbrani tako, da študentom omogočajo celovit in zaokrožen opis sintetiziranih spojin. Eksperimentalne vaje potekajo v skupinah z dvema do štirimi študenti ob mentorstvu učitelja ali asistenta.	General contents will be processed by lectures and seminars, practical exercises in laboratory. Content of lab work: Synthesis of coordination compounds based on known literature data, followed by their detailed characterization with the spectroscopic , the magnetic susceptibility and the electrical conductivity methods. Practical methods include applying of X-ray powder diffraction, infra-red and UV-visible spectroscopy, magnetic susceptibility and electrical conductivity. Additionally, electron spin and nuclear magnetic resonance method (EPR, NMR) are presented to students. Characterization methods and compound examples are selected so that students can completely and thoroughly describe the synthesized compounds. Experiments are conducted in groups of two to four students with the assistance of a teacher or an assistant.

Temeljna literatura in viri / Readings:

J. D. Lee, Concise Inorganic Chemistry, Chapman and Hall, 5. Izd. 1996, 7., 32. poglavje.
B. Kozlevčar, Koordinacijska kemija, Navodila za vaje, študijsko gradivo, UL FKKT, 2013.
Dopolnilna literatura /additional readings:
A. K. Brisdon, Inorganic Spectroscopic Methods, Oxford Univ. Press, 1993.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Načrtovanje projekta, ki obsega iskanje literature za sintezni postopek, sintezo spojine, njeno analizo ter vrednotenje rezultatov s preverjanjem ujemanja rezultatov s podatki, navedenimi v objavljeni literaturi - Podrobnejša uporaba metod, primernih za karakterizacijo koordinacijskih spojin -Predstavitev in prikaz metod, ki so pri rutinski manj uveljavljene in se jih redkeje uporablja *Kompetence:* Študenti bi začrtane naloge opravili z čim večjo mero samostojnosti, kar predstavlja dejanski prehod med opravljanjem in reševanjem preprostejših izzivov, s katerimi se srečajo na osnovnem nivoju študija ter popolno samostojnostjo, ki se na ustreznem delovnem mestu pričakuje od človeka z zaključeno magistrsko stopnjo izobrazbe.	Planning of the project comprising searching of literature for the synthesis process, the synthesis of compounds, their analysis and evaluation of the results by checking the correlation of the results with the data specified in the published literature. - A detailed methods application, suitable for the characterization of coordination compounds -Presentation and display of the methods not routine, less established and not widely used Students shell outline the tasks performed by the largest possible autonomy, representing actual transition between the performance and the handling of simple challenges facing on a basic study level and the complete independence, which is at a specific working place expected for a person with the master's degree.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Študenti so sposobni samostojno načrtovati sintezno shemo spojine, jo potem izpeljati in sintetizirano koordinacijsko spojino natančno okarakterizirati. Imajo pregled nad dosegljivimi metodami in znajo oceniti njihovo uporabnost.	Knowledge and Comprehension Students are independently able to design the coordination compounds synthesis scheme, perform the syntheses and accurately characterize them. Show an overview of the accessible methods and know how to evaluate their applicability**.**
Uporaba Strukturiranje izvedbe projekta je namenjeno predvsem reševanju zahtevnejših nalog, s katerimi se kemik pogosto sreča pri nadaljevanju študija ali v poklicu. Potek od želje po izolaciji spojine in uporabe postopkov za njeno karakterizacijo ter morebitno ocene njene praktične uporabnosti je pogosto zahteven in dolgotrajen. Metode, ki jih študentje srečajo in uporabljajo pri tem predmetu, so relativno pogosto uporabne in omogočajo razne analize, od rutinskih do bolj specifičnih.	Application The project execution is structuring primarily to complex tasks solving design, a chemist often meets at further studies or professional careers. The procedure from a desire for a compound isolation and its characterization and assessment of its potential practical application is often difficult and time consuming. The methods students meet and apply in this course are relatively often used thus enabling various analyses, from routine to more specific.
Refleksija Pridobljena znanja bodo študentu omogočila analizo izzivov pri reševanju nalog, s katerimi se bo srečeval v laboratoriju. Uporabil bo lahko primerno metodo, jo samostojno izpeljal ali celo vodil skupino ljudi pri določenem delovnem procesu.	Analysis The acquired knowledge will enable students to analyse the challenges at tasks addressing, which will be encountered in the laboratory. The appropriate method will be chosen, carried out independently or even as a group leader in a particular working process.
Prenosljive spretnosti Po končanem študiju bo izpeljava začrtane naloge na osnovi postavitve načrta izvedbe tista bistvena sposobnost, ki se od študenta pričakuje Skupaj z znanjem, potrebnim za iskanje primernih virov informacij, nujnih pri izvedbi delovnih postopkov na določenem delovnem mestu, bo to morda največja prednost takšne osebnosti.	Skill-transference Ability A derivation of the planned tasks, base on the set plan, shell be the essential skill, one would expect from the student after the graduation. Along with the knowledge needed to find appropriate information sources, being necessary at the work processes execution at the specific working place, this may be the largest advantage of such personalities.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Projektno delo v manjših skupinah.	Seminar and laboratory project work in small groups

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

Pisni izpit po uspešno opravljenem praktičnem delu. Ocene: pozitivno 6-10		Written exam after practical work successfully completed. Positive grades 6-10

Reference nosilca / Lecturer's references:

- KOZLEVČAR, Bojan, GAMEZ, Patrick, GELDER, René de, JAGLIČIĆ, Zvonko, STRAUCH, Peter, KITANOVSKI, Nives, REEDIJK, Jan. Counterion and solvent effects on the primary coordination sphere of copper(II) bis(3,5-dimethylpyrazol-1-yl)acetic acid coordination compounds. Eur. J. Inorg. Chem., 2011, 3650-3655, doi: 10.1002/ejic.201100410. [COBISS.SI-ID 35234309]
- KOZLEVČAR, Bojan, ŠEGEDIN, Primož. Structural analysis of a series of copper(II) coordination compounds and correlation with their magnetic properties. Croat. Chem. Acta, 2008, 81, 369-379, [COBISS.SI-ID 29994501]
- KOZLEVČAR, Bojan, LEBAN, Ivan, PETRIČ, Marko, PETRIČEK, Saša, ROUBEAU, Olivier, REEDIJK, Jan, ŠEGEDIN, Primož. Phase transitions and antiferromagnetism in copper(II) hexanoates : a new tetranuclear type of copper carboxylate paddle-wheel association. Inorg. Chim. Acta, 2004, 357, 4220-4230, [COBISS.SI-ID 1184649]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MAGISTRSKO DELO
Course Title:	MASTER'S THESIS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	**/**	**2.**	**3. in 4.**
USP Chemistry, 2nd Cycle	**/**	**2nd**	**3rd and 4th**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE223

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
/	**/**	**/**	**/**	**450**	**/**	**30**

Nosilec predmeta / Lecturer: /

Jeziki / Languages: **Predavanja / Lectures:** **/**
Vaje / Tutorial: **/**

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):
Magistrsko delo se opravlja na področju kemije. Vsebina in naslov se določata v soglasju z izbranim mentorjem – nosilcem ene izmed vsebin v programu.	Master's thesis is performed in one of the areas of chemistry. Contents and Master's thesis title are agreed upon with the mentor.

Temeljna literatura in viri / Readings:

Knjige in članki, ki so povezani z vsebino magistrskega dela.
Books and journal articles related to the research topic.

Cilji in kompetence:	Objectives and Competences:
Cilj: Dokončno oblikovanje pričakovanega lika magistranta. Študent bo ob izdelavi magistrske naloge pokazal sposobnosti iskanja in zaznavanja kemijskih problemov in znal poiskati rešitev za tak problem.	Final formation of the competences of a master's degree candidate; Through carrying out research for the master's thesis students should be able to demonstrate the skills for autonomous identification of a problem and

Kompetence: Pri delu bo pokazal, da je pridobil večino kompetenc navedenih v programu študija.	finding solutions, thus proving that specific competences from other courses have been acquired.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Pri izdelavi magistrskega dela bo slušatelj pridobil: • sposobnosti formuliranja problema, • sposobnosti samostojnega iskanja ustrezne literature, • sposobnosti obravnavanja problema v praksi, • sposobnosti iskanja kvantitativnih rešitev in utemeljevanja ustreznosti rešitev, sposobnosti predstavitve rezultatov svojega dela.	Knowledge and Comprehension Ability to formulate the problem and research literature independently; Ability of independent problem managing in practice; Ability of independent quantitative problem solving and argumentation of the solution; Ability of presenting results of research work.
Uporaba Znanje in pridobljene veščine bo magistrant lahko uporabil pri opravljanju poklica.	Application Acquired skills are necessary for professional work.
Refleksija Povezovanje vseh pridobljenih teoretičnih znanj z reševanjem problemov na področju kemije ter kritični pogled na uporabnost teh znanj.	Analysis Integration of knowledge from different topics from chmistry and supporting sciences; Development of a critical view on the knowledge applicability.
Prenosljive spretnosti Pri delu bo magistrant pridobil znanja o metodah reševanja kompleksnih problemov, o načinu prezentacije teh znanj v pisani in govorjeni obliki, povezani z ostalimi metodami posredovanja raziskav, ugotovitev itd.	Skill-transference Ability Ability of solving complex problems using different methods; Ability of presenting research results in a written and oral form.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Individualno delo mentorja in samostojno študijsko in raziskovalno delo.	Independent research work supervised by the mentor.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	Assessment:
Ocenjuje se magistrsko delo (50 %) in zagovor magistrskega dela (50 %). Komisijo sestavljajo predsednik, mentor in član. Lestvica ocen vsakega dela je od 1 do 10. Ocene 1 do 5 so negativne, ocene 6 do 10 pa pozitivne in sicer: 6-- zadostno, 7-- dobro, 8 in 9-- prav dobro, 10--odlično		Master's thesis and its presentation are graded separately by a three-member commission (chairman, mentor, additional member) against the grading scale from 1- 10 (grades from 6 – 10 are positive and 1 -5 negative (6-pass, 7-fair, 8 and 9-very good, 10-excellent).

Reference nosilca / Lecturer's references:

/

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MATEMATIKA II
Course Title:	MATHEMATICS II

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

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: K2123

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

Nosilec predmeta / Lecturer: izr. prof. dr. Jasna Prezelj / Dr. Jasna Prezelj, Associate Professor
prof. dr. Bojan Magajna / Dr. Bojan Magajna, Full 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):
Dvojni in trojni integral: definicija in osnovne lastnosti (najprej za dvojni integral), računanje integralov v kartezičnih, polarnih cilindričnih in sferičnih koordinatah, primeri, dolžine krivulj, površine ploskev in prostornine teles, delo in pretok vektorskega polja, Gaussov in Stokesov izrek. **Fourierove vrste:** Hilbertovi prostori, prostori funkcij kot Hilbertovi prostori, baza prostora, ortogonalnost in ortonormiranost, periodične funkcije reševanje enačbe nihanja strune in	Double and triple integral: definition and basic properties, Cartesian, polar, cylindrical and spherical coordinates, examples, length of a curve, area and volume, flux and work, Gauss and Stokes theorem. Fourier series: scalar product, spaces of functions with scalar product (Hilbert space), orthonormal base, periodic functions, examples of trigonometric orthonormal bases, examples of Fourier expansions, applications to wave and heat equation, eigenfunctions. Fourier transform: derivation of the transform from Fourier series and inverse formula, basic properties, convolution, inverse formula, unitariness, applications: heat, wave and time

toplotne enačbe, lastne funkcije), Fourierove vrste. **Fourierova transformacija:** prehod od Fourierove vrste do Fourierove transformacije in inverzna formula, razumevanje koncepta Fourierove transformiranke, osnovne lastnosti, konvolucija, unitarnost, uporaba pri reševanju nekaterih parcialnih diferencialnih enačb (toplotna enačba, od časa neodvisna Schroedingerjeva enačba) **Verjetnost in statistika**: osnovni pojmi, pogojna verjetnost, neodvisni dogodki in poskusi, Bernoullijevo zaporedje, slučajne spremenljivke (zvezne in diskretne) in porazdelitvene funkcije, dvorazsežne porazdelitve, pričakovana vrednost in varianca, korelacija, zakon velikih števil, enostavno slučajno vzorčenje	independent Schroedinger equation. Probability: basic notions, conditional probability, Bernoulli trials, discrete and continuous random variables, one and two dimensional distribution functions, examples, expected value, variance, correlation, law of large numbers, simple random sampling.

Temeljna literatura in viri / Readings:

1. Josip Globevnik in Miha Brojan: Analiza II, FMF, 2012 (Poglavje dvojni in trojni integral).
2. Anton Suhadolc: Metrični prostor, Hilbertov prostor, Fourierova analiza, Laplaceova transformacija, DMFA 1998 (poglavji Fourierove vrste in Fourierova transformacija).
3. Milan Hladnik: Verjetnost in statistika, Založba FE in FRI, 2002 (poglavje Verjetnost in statistika)

Dopolnilna literatura:

1. P. Mizori-Oblak: Matematika za študente tehnike in naravoslovja, 2. Del FS, 1997.
2. H. P. Greenspan, D.J. Benney / J.E. Turner: Calculus: an introduction to applied mathematics, McGraw-Hill, Toronto, 1986
3. Rajko Jamnik: Matematika, DMFA Slovenije, 1994.
4. Bojan Magajna, http://www.fmf.uni-lj.si/~magajna/Matematika2KEM/osnovna.htm

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta: Seznaniti študente z nekaterimi pojmi in metodami matematične analize in verjetnostnega računa, ki jih naravoslovec pogosto potrebuje pri svojem delu in omogočajo boljše razumevanje drugih strokovnih predmetov. *Predmetno specifične kompetence:* Pridobljeno znanje bo študentu omogočilo globlje razumevanje nekaterih področij kemije. Na primer, dobrega razumevanja	Objectives: students are acquainted with notions and methods of mathematical analysis and probability theory that are often used by scientists and help in understanding other subjects. Competences: better understanding of some topics in chemistry, for example the structure of the atoms cannot be well understood without basics in Hilbert space techniques.

strukture atomov in molekul (ali pa določenih tehnoloških procesov) si ni mogoče zamisliti brez ustreznega znanja matematike, ki vključuje celotno vsebino predmeta.	

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Razširiti znanje in poglobiti razumevanje pridobljeno pri predmetih matematika 1 in matematika 2 ter spoznati nove matematične metode, uporabne v drugih znanostih.	Knowledge and Comprehension Extending knowledge and widening comprehension of mathematics acquired in the courses Mathematics I and II, learning new methods that are applicable to chemistry.
Uporaba V naravoslovju (npr. verjetnosti v kinetični teoriji plinov, Fourierove transformacije v kvantni fiziki in kemiji...)	Application Probability is used in the theory of gasses, Fourier transform in quantum physics and chemistry and so on.
Refleksija Kljub abstraktni naravi, je tematika predmeta zelo uporabna pri konkretnih problemih iz kemije ali fizike, tako da je na mnogih univerzah to obvezen del programa študija kemije.	Analysis The mathematics contained in the proposed course is useful in studying problems in chemistry and physics.
Prenosljive spretnosti Znanje, ki ga nudi predmet, je osnova za boljše razumevanje vsebin nekaterih drugih predmetov in (na primer) za uspešno uporabo računalniških modelov v znanosti in tehnologiji.	Skill-transference Ability The acquired knowledge is basic for a better understanding of other courses and application of computer modelling in science and technology.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, vaje, sodelovalno učenje /poučevanje.	Lectures, tutorial, homework, consultations

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
(a) kolokviji, pisni izpiti, ustni izpiti. (b) domače seminarske naloge, če se bo to pokazalo za potrebno in koristno. Od 6-10 (pozitivno) oz. 1-5 (negativno) oz. opravil/ ni opravil; ob upoštevanju Statuta UL in fakultetnih pravil.		(a) Written examination, oral examination (b) Seminar if necessary Grading: 6 – 10 (positive), 1 -5 (negative)

Reference nosilca / Lecturer's references:

1. J. Prezelj: Weakly holomorphic embeddings of Stein spaces with isolated singularities, Pacific

Journal of Mathematics 220 (1): (2005) 141--152
2. F. Forstnerič, B. Ivarsson, F. Kutschebauch, J. Prezelj: An interpolation theorem for proper holomorphic embeddings, Math. Ann. 338 (2007), 545--554
3. J. Prezelj: A relative Oka-Grauert principle for holomorphic submersions over 1-convex spaces, Trans. Amer. Math. Soc. 362 (2010), 4213-4228.

1. B. Magajna: Bicommutants and ranges of derivations. *Linear and Multilinear Algebra*, ISSN 0308-1087, 2013, vol. 61, no. 9, str. 1161-1180.
2. B. Magajna: . Sums of products of positive operators and spectra of Lüders operators. *Proceedings of the American Mathematical Society*, ISSN 0002-9939, 2013, vol. 141, no. 4, str. 1349-1360.
3. M. Brešar, B. Magajna, Š. Špenko: Identifying derivations through the spectra of their values. *Integral equations and operator theory*, ISSN 0378-620X, 2012, vol. 73, no. 3, str. 395-411.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	METODE SIPANJA ZA DOLOČANJE STRUKTURE IN DINAMIKE V NANOSISTEMIH
Course Title:	METHODS OF SCATTERING FOR DETERMINING STRUCTURE AND DYNAMICS IN NANOSYSTEMS

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: K2I20

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. Andrej Jamnik / Dr. Andrej Jamnik, Full 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):
Uvod v metode sipanja Lorentzov model. Lorentzova limita in limita sipanja. Interferenca. **Ozkokotno rentgensko sipanje** (metoda SAXS) Rayleigh-Debye-Gansova (RDG) teorija. Sipanje in inverzni problem sipanja. Razredčeni monodisperzni sistemi. Radij giracije, molska masa. Indirektna Fourierova transformacija - metoda IFT. Parska porazdelitvena funkcija razdalj. Notranja struktura delcev. Koncentrirani sistemi. Posplošena indirektna Fourierova transformacija – metoda GIFT. Eksperimentalni sistem. Aplikacije metode SAXS. Osnove ozkoktnega nevtronskega sipanja: kontrast in variacija kontrasta,	**Introduction to scattering methods** Lorentz model. Lorentz limit and scattering limit. Interference. **Small-angle X-ray scattering** (SAXS method) Rayleigh Debye Gans (RDG) theory. Scattering problem and inverse scattering problem. Dilute monodisperse systems. Radius of gyration, molar mass. Indirect Fourier transformation (ITP method). Pair distance distribution function. Internal structure of particles. Concentrated systems. Generalized indirect Fourier transformation (GIFT method). Experimental setup. Applications of SAXS method. Basic of small-angle neutron scattering (SANS method). Contrast variation. Selective deuteration.

selektivno devteriranje. **Statično sipanje laserske svetlobe** (metoda SLS) Rayleighovo sipanje, RDG področje. Teorija fluktuacij za razredčene sisteme. Zimmov diagram. Monodisperzni in polidisperzni sistemi. Eksperimentalni sistem. **Dinamično sipanje laserske svetlobe** (metoda SLS) Difuzija in hidrodinamski radij delcev. Avtokorelacijska funkcija. Koncentracijski efekti. Inverzna Laplaceova transformacija avtokorelacijske funkcije. Rotacijski difuzijski koeficient. Ergodijski in neergodijski sistemi. **Laboratorijske vaje** Projektne vaje: Strukturne raziskave izbranih nano-strukturiranih sistemov z metodami SAXS, SLS in DLS – izvedba eksperimentov ter analiza in interpretacija meritev sipanja.	**Static light scattering** (SLS method) Rayleigh scattering. RDG domain. Fluctuation theory for dilute systems. Zimm plot. Monodisperse and polydisperse systems. Experimental setup. **Dynamic light scattering** (DLS method) Diffusion coefficient and hydrodynamic radius of particles. Autocorrelation function. Concentration effects. Inverse Laplace transformation of autocorrelation function. Rotation diffusion coefficient. Ergodic and non-ergodic (arrested) systems. **Project works** Structural investigation of chosen nano-systems by SAXS, SLS and DLS – performing experiments and analysis and interpretation of experimental data.

Temeljna literatura in viri / Readings:

- O. Glatter in O. Kratky, Small Angle X-Ray Scattering, Academic Press, 2. izdaja (1983), 30 % od 510 str., ISBN 0-12-286280-5
- B. J. Berne in R. Pecora, Dynamic Light Scattering: With Application to Chemistry, Biology, and Physics, Dover Publications (2000), 20 % od 372 str., ISBN 978-0-486-41155-2

Dopolnilna literatura

- P. Lindner in T. Zemb, Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter, Elsevier (2002), 541 str., ISBN 0-444-51122-9
- R. J. Roe, Methods of X-Ray and Neutron Scattering in Polymer Science, Oxford University Press (2000), 315 str., ISBN 978-0-19-511321-1
- A. Jamnik, Metode sipanja za določanje strukture in dinamike v nanosistemih, zapiski predavanj.

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta je spoznavanje različnih eksperimentalnih metod, ki temeljijo na sipanju rentgenskih žarkov in nevtronov pod majhnimi koti ter sipanju laserske svetlobe. Te metode se uporabljajo za določevanje strukturnih in dinamičnih značilnosti nanosistemov. Študenti si pri predmetu pridobijo naslednje specifične *kompetence:* - razumevanje teorijskega ozadja sipanja svetlobe - pridobitev eksperimentalnih veščin za	The aim of the course is to learn the different experimental methods, which are based on the small-angle scattering of X-rays and neutrons, and laser light scattering. These methods are used to determine the structural and dynamic characteristics of nanosystems. Students of the course gain the following specific competences: - Understanding the theoretical background of light scattering - The acquisition of skills for the experimental measurement of small-angle scattering and

merjenje ozkokotnega rentgenskega sipanja ter statičnega in dinamičnega sipanja laserske svetlobe - sistematičnost pristopa pri reševanju projektne naloge - uporaba računalniške programske opreme za analizo meritev sipanja - usposobljenost za samostojno reševanje projektnih nalog in za izdelavo poročil	static and dynamic laser light scattering - A systematic approach to dealing with project tasks - The use of computer software for the analysis of experimental data - Ability to independently solve project tasks and to write scientific reports

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Osnovno teorijsko znanje o interakciji elektromagnetnega valovanja (vidna svetloba, rentgenski žarki) s snovjo. Razumevanje pojava sipanja na posameznih sipalnih centrih ter interference sekundarnih valov. Razumevanje pojmov, ki se uporabljajo pri teorijskih obravnavah sipanja, in zakonitosti, ki sledijo iz teh obravnav. Poznavanje eksperimentalnih sistemov za merjenje rentgenskega in laserskega sipanja. Poznavanje numeričnih metod za obdelavo in interpretacijo meritev sipanja ter možnih zaključkov o strukturnih parametrih, ki sledijo iz te analize.	Knowledge and Comprehension Basic theoretical knowledge of the interaction of electromagnetic radiation (visible light, X-rays) with the matter. Understanding the phenomenon of scattering on the individual scattering centres and the interference of secondary waves. Understanding of the concepts used in theoretical treatments of scattering, and of general laws, which follow from these treatments. Knowledge of the experimental system for measuring the X-ray and laser scattering. Knowledge of numerical methods for the data treatment and interpretation of experimental data, and of possible conclusions about the structural parameters that follow from this analysis.
Uporaba Uporaba metod sipanja za določitev strukturnih in dinamičnih lastnosti zelo različnih sistemov, pri katerih gre za notranjo strukturiranost v koloidnem (nano) območju dimenzij (biološki sistemi - proteini, nukleinske kisline, membrane, makromolekule, polimeri, surfaktanti, mikroemulzije).	Application The use of scattering methods to determine the structural and dynamic properties of very different systems which show internal structure of colloidal (nano) dimensions (biological systems - proteins, nucleic acids, membranes, macromolecules, polymers, surfactants, microemulsions).
Refleksija Občutek za povezavo med splošno teorijo in modelnimi izračuni sipanja, ki iz te sledijo, ter eksperimentalnimi rezultati. Kritično ovrednotenje rezultatov, ki sledijo iz numerične analize meritev sipanja.	Analysis Connection between the general scattering theory and model calculations that follow from this theory, and the experimental results. Critical evaluation of the results arising from the numerical analysis of experimental scattering data.

Prenosljive spretnosti	Skill-transference Ability
Zbiranje in uporaba znanstvenih člankov pri projektnem (raziskovalnem) delu. Poročanje o predelani literaturi, predstavitev rezultatov projektnih vaj, ter pisanje poročila v obliki znanstvenega članka.	Collection and use of scientific articles in the project research work. Reporting on the used literature, presentation of the results of project work and report writing in the form of a scientific article.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji, projektne laboratorijske vaje.	Lectures, seminars, and laboratory practice.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
- Pisni izpit - Predstavitev rezultatov projektnih vaj Ocenjevanje: 6-10 (pozitivno); 1-5 (negativno).	50 50	- Written examination - Presentation of the results of project practical work Marks: 6-10 (positive); 1-5 (negative).

Reference nosilca / Lecturer's references:

- J. Orehek, I. Dogša, M. Tomšič, A. Jamnik, D. Kočar, D. Stopar, Structural investigation of carboxymethyl cellulose biodeterioration by *Bacillus subtilis* subsp*. subtilis* NCIB 3610, Int. Biodeterioration & Biodegradation 77, 2013, 10-17.
- A. Vrhovšek, O. Gereben, A. Jamnik, L. Pusztai, Hydrogen bonding and molecular aggregates in liquid methanol, ethanol, and 1-propanol, J. Phys. Chem. B 115, 2011, 13473-13488.
- A. Lajovic, M. Tomšič, G. Fritz-Popovski, L. Vlček, A. Jamnik, Exploring the structural properties of simple aldehydes: A Monte Carlo and small-angle x-ray scattering study, J. Phys. Chem. B 113, 2009, 9429-9435.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MODELIRANJE KEMIJSKIH SISTEMOV
Course Title:	MODELLING OF CHEMICAL SYSTEMS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	/	2.	4.
USP Chemistry, 2nd Cycle	/	2nd	4th

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I22

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

Nosilec predmeta / Lecturer: izr. prof. Tomaž Urbič / Dr. Tomaž Urbič, Associate Professor

Jeziki / Languages:

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

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):
Ponovitev osnov o programskih jezikih (fortran, c, phyton, java), ki se bodo predvidoma uporabljali za praktično delo na računalniku. Statistične metode in pristopi pri obdelavi eksperimentalnih podatkov. Modeliranje podatkov (aproksimacija z nelinearnimi funkcijami). Filtriranje signalov in interpretacija (IR, NMR, masnih) spektrov (Fourierova transformacija in Fourierova analiza). Izračun časovnega poteka kemijskih reakcij (kemijska kinetika). Modeliranje dvoelektronskih sitemov v Hartree-Fockovem približku, primer helijevega atoma in vodikove molekule. Predstavitev in reševanje difuzijskih	Introduction in basics of computer programming (fortran, c, python, java) which will be used in practical work on computers. Statistical methods for representation of experimental data. Modelling of data (fitting with non-linear functions). Filtering of signals and interpretation of (IR, NMR, mass) spectra (Fourier transform and Fourier analysis). Time dependence of chemical reactions (chemical kinetics). Modelling of two-electron systems with Hartree-Fock approximation (helium atom and hydrogen molecule). Numerical approximations for solving of partial differential equations (diffusion problems, flow of fluids and flow of heat). Lattice Boltymann method. Calculation of structure of fluids and solutions

problemov, pretakanja tekočin in toplotnih sistemov (numerično reševanje parcialnih diferencialnih enačb). Lattice Boltzmannova metoda. Določanje strukture tekočin in raztopin s pomočjo reševanja integralskih enačb. Modeliranje slučanih procesov. Numerično integriranje s pomočjo Monte Carlo metode in Monte Carlo simulacije preprostih tekočin (Metropolisov algoritem). Molekulska dinamika preprostih kemijskih sitemov.	by integral equation theory. Modelling of coincidental events. Numerical integration with Monte Carlo method and Monte Carlo simulation of simple fluids (Metropolis algorithm). Molecular dynamics of simple chemical systems.

Temeljna literatura in viri / Readings:

-W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Numerical Recipes in Fortran, Cambridge University Press, Cambridge, 1994. (20%)
-D. Frenkel, B. Smit, Understanding Molecular Simulation, Academic Press, San Diego, 1996. (10%)
-Priročniki za programske jezike.

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta je študentom predstaviti metode za numerično reševanje matematičnih problemov, na katere lahko naleti pri vsakdanjem delu na področju znanosti, tehnike. *Kompetence:* Pri predmetu naj bi dobil študent teoretično podlago in praktične izkušnje za samostojno reševanje matematičnih problemov, na katere naleti pri vsakodnevnem delu na različnih področij znanosti in tehnike s posebnim poudarkom na kemijo.	Goal: To understand basic numerical methods for solving of mathematical problems which scientists can find in everyday work in science and technology. Competence: Students will get theoretical and practical experience to independently solve mathematical problems which can be found at everyday work in different field of science and technology with emphasis on chemistry.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Predmet je namenjen seznanjanju z osnovnimi metodami za reševanje numeričnih problemov v naravoslovju in tehniki s posebnim poudarkom na kemiji. Študent se nauči identificirati problem, ga razčleniti in potem rešiti s pomočjo računalniškega programa.	<u>Knowledge and Comprehension</u> Goal of the subject is to acquaint students with basic methods for solving numerical problems in science and technology with emphases on chemistry. Student will learn how to identify problem, examine it and later solve it with help of computer program.
<u>Uporaba</u> Uporabnost pridobljenega znanja je zelo široka in nikakor ni omejena samo na fizikalno kemijo oziroma kemijo. Študent se je sposoben spoprijeti skoraj z vsakim numeričnim problemom, na katerega naleti	<u>Application</u> Usefulness of gained knowledge is very general and goes beyond physical chemistry and chemistry. Student gets knowledge that he can use to solve any kind of numerical problem he might find during the study and later in any kind

med študijem ali pozneje, neodvisno od področja znanosti.	of field of science.
Refleksija Študent pridobi občutek, da se je sposoben lotiti poljubnega problema in si pri tem pomagati z računalniškimi programi.	Analysis Student gets the feeling that he is capable of solving any kind of problem with help of computer programming.
Prenosljive spretnosti Spretnosti in znanje, ki si ga študent pridobi pri predmetu, so v največji meri splošne in prenosljive, uporabne na vseh področjih znanosti in tehnike, kjer si lahko pri reševanju problemov pomaga z računalnikom.	Skill-transference Ability Knowledge and experience are general and can be used in all areas of science and technology, where one can find problems that can be solved with help of computer.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji, praktične vaje na računalniku.	Lectures, seminars and practical work on computers.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
- projekt - seminarske in domače naloge Ocene: 6-10 (pozitivno), 1-5 (negativno) ob upoštevanju Statuta UL in fakultetnih pravil.	**50** **50**	- final project - seminars and homeworks Grades: 6-10 (pozitive), 1-5 (negative)

Reference nosilca / Lecturer's references:

- URBIČ, Tomaž, VLACHY, Vojko, KALYUZHNYI, Yu. V., SOUTHALL, N. T., DILL, K. A. A two dimensional model of water : theory and computer simulations. J. chem. phys., February 2000, vol. 112, no. 6, str. 2843-2848.
- URBIČ, Tomaž, BEŠTER-ROGAČ, Marija, JAMNIK, Andrej, STARE, Jernej. Small-angle x-ray scattering functions of rodlike polyelectrolytes in aqueous solutions. Acta chim. slov.. [Tiskana izd.], September 2001, vol. 48, 343-352.
- URBIČ, Tomaž, VLACHY, Vojko, KALYUZHNYI, Yu. V., DILL, K. A. Orientation-dependent integral equation theory for a two-dimensional model of water. J. chem. phys., 2003, 118, 5516-5525.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MODERNE METODE ORGANSKE SINTEZE
Course Title:	MODERN METHODS OF ORGANIC SYNTHESIS

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, 2nd Cycle	/	1st	2nd

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I09

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

Nosilec predmeta / Lecturer: prof. dr. Jurij Svete / Dr. Jurij Svete, Full 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:

Uvod: Moderni trendi v organski sintezi. Klasična organska sinteza: kratek pregled, zmožnosti, omejitve in metode povečanja učinkovitosti.
Reagenti v organski sintezi. Tvorba C–C, C–H, C–X, C=C in C=X vezi v organski sintezi: pregled reagentov v metodah alkiliranja, olefiniranja, ariliranja, aciliranja, halogeniranja, hidroksiliranja, aminiranja, oksidacije in redukcije. Organo-S,Si,P,B reagenti. Organokovinski reagenti.
Načrtovanje organskih sintez. Retrosintezna analiza. Sintoni in sintezni ekvivalenti.
Kemoselektivnost in regioselektivnost. Pregled značilnih pravokotnih setov s primeri najpogosteje uporabljanih zaščitnih skupin.
Stereoselektivnost. Osnovni principi stereoselektivne in asimetrične sinteze. Stereoselektivne nekatalitske reakcije. Asimetrične katalitske reakcije in asimetrična organokataliza.

Content (Syllabus outline):

Introduction: Modern trends in organic synthesis. Classical organic synthesis: survey, scope and limitations, methods for efficacy improvement.
Reagents in organic synthesis. Formation of C–C, C–H, C–X, C=C, and C=X bond in organic synthesis: survey on reagents for alkylation, olefination, arylation, acylation, halogenation, hydroxylation, amination, oxidations, and reductions. Organo-S,Si,P,B reagents. Organometallic reagents.
Planning organic syntheses. Retrosynthetic analysis. Synthons and synthetic equivalents.
Chemoselectivity and regioselectivity. Survey on typical orthogonal sets with examples of the most commonly used protecting groups.
Stereoselectivity: Basic principles of stereoselective and asymmetric synthesis. Stereoselective non-catalytic reactions. Asymmetric catalytic reactions, asymmetric organocatalysis.

Večkomponentne in tandemske (domino, kaskadne) reakcije. **Principi kombinatorne sinteze.** Kombinatorna sinteza na polimernih nosilcih. Tipični polimerni nosilci, distančniki in vezniki. Kombinatorna sinteza v raztopini. Reagenti in izolacijske tehnike pri kombinatorni sintezi v raztopini. **Avtomatizacija laboratorijskih tehnik v organski sintezi.** Izvedba in spremljanje reakcij. Izolacijske tehnike. Karakterizacija.	**Multicomponent and tandem (domino, cascade) reactions.** **Principles of combinatorial synthesis:** Solid-phase combinatorial synthesis. Typical polymer supports, linkers, and spacers. Solution-phase combinatorial synthesis. Reagents and isolation techniques in solution-phase combinatorial synthesis. **Automation of laboratory techniques in organic synthesis .** Reaction performing and monitoring. Isolation techniques. Compound characterisation.

Temeljna literatura in viri / Readings:

J. Clayden, N. Graves, S. Warren: *Organic Chemistry, 2nd Edition*, Oxford University Press, 2012, 1264 strani; ca. 15% (ca. 170 pages) and selected topics from synthetic organic chemistry (23, 24, 28, 32, 33, 41, 43).

Dodatna literatura / Supplementary Readings:

J.-H. Führhop, G. Li, *Organic Synthesis Concepts and Methods*, 3rd, completely revised and enlarged Edition, Wiley-VCH, Weinheim, 2003, 517 pages (selected topics).

W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, Cambridge, 2004, 506 pages (selected topics).

Review articles covering selected topics on synthetic chemistry (recent papers published in the last decade).

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta: -poznavanje modernih pristopov k sintezi organskih spojin in sodobnih trendov na tem področju -poznavanje principov stereoselektivne, asimetrične in kombinatorne sinteze -poznavanje večkomponentnih in tandemskih reakcij ter 'klik' kemije in njihove uporabe v moderni organski sintezi -poznavanje modernih eksperimentalnih metod, tehnik in reagentov v organski sintezi *Predmetno specifične kompetence*: -načrtovanje organskih sintez: kreiranje nabora možnih sinteznih poti in racionalna izbira najprimernejše poti, -izbira ustreznih sinteznih metod in tehnik in izbira reagentov, -načrtovanje in izvedba usmerjene oz. ciljne sinteze, -načrtovanje in sinteza kombinatornih knjižnic.	***Objectives:*** - Knowledge on modern approaches in organic chemistry. - Knowledge on principles of stereoselective, asymmetric, and combinatorial chemistry - Knowledge on multicomponent and tandem reactions and 'click' chemistry and their application in modern organic synthesis - Knowledge on modern experimental methods, techniques, and reagents in organic synthesis ***Competences:*** - Planning of organic syntheses: elaboration of possible synthetic routes and rational choice of the most suitable synthetic approach - Choice of suitable synthetic methods, techniques, and reagents - Planning directed and target syntheses - Planning and synthesis of combinatorial libraries

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje **Znanje:** -klasične in moderne metode v organski sintezi -načrtovanje in izvedba sintez organskih spojin **Razumevanje:** -splošnih principov moderne organske sinteze -principov stereoselektivne, asimetrične in kombinatorne sinteze	Knowledge and Comprehension Knowledge*:* - classical and modern methods in organic synthesis - planning and performance of the syntheses of organic compounds Comprehension: - general principles of modern organic synthesis - principles of stereoselective, asymmetric, and combinatorial synthesis
Uporaba Racionalno načrtovanje in praktična izvedba organskih sintez (usmerjene in ciljne sinteze organskih spojin in sinteze kombinatornih knjižnic).	Application Rational planning and practical performance of organic syntheses (directed and target synthesis of organic compounds and the synthesis of combinatorial libraries)
Refleksija Študent bo na osnovi pridobljenega znanja sposoben načrtovati sintezo enostavnih in kompliciranih organskih spojin in nato primerjati in kritično ovrednotiti možne sintezne poti. Na podlagi pridobljenega znanja se bo spodoben odločiti za najbolj racionalno sintezno pot in jo tudi preizkusiti v praksi.	Analysis On the basis of the acquired knowledge, the student is able to plan the synthesis of simple and complex organic compounds and to critically evaluate possible synthetic pathways. The student is able to choose and practically evaluate the most suitable (rational) synthetic approach.
Prenosljive spretnosti -Dostopanje do literaturnih virov -Zbiranje, interpretacija in kritično vrednotenje podatkov -Identifikacija in reševanje problemov -Poročanje (pisno in ustno) **-**Kritična analiza, sinteza	Skill-transference Ability - access to and the use of literature sources - collection, interpretation, and critical data evaluation - identification and solving the problems - reporting and presentation of the results (oral and written) - critical analysis and synthesis

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji in vaje	Lectures, seminars, seminar projects, and laboratory trainings

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminarska naloga, ustni izpit. Ocene: 6-10 (pozitivno), 1-5 (negativno)	**30 %** **70 %**	Seminar work, oral exam Grades: 6-10 (positive), 1-5 (negative)

Reference nosilca / Lecturer's references:

- BAŠKOVČ, Jernej, DAHMANN, Georg, GOLOBIČ, Amalija, GROŠELJ, Uroš, KOČAR, Drago, STANOVNIK, Branko, SVETE, Jurij. Diversity-oriented synthesis of 1-substituted 4-aryl-6-oxo-1,6-dihydropyridine-3-carboxamides. *ACS combinatorial science*, ISSN 2156-8952, 2012, vol. 14, no. 9,

str. 513-519, doi: 10.1021/co3000709. [COBISS.SI-ID 36122373]
- MALAVAŠIČ, Črt, BRULC, Blaž, ČEBAŠEK, Petra, DAHMANN, Georg, HEINE, Niklas, BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Combinatorial solution-phase synthesis of (2S,4S)-4-acylamino-5-oxopyrrolidine-2-carboxamides. *Journal of combinatorial chemistry*, ISSN 1520-4766, 2007, vol. 9, no. 2, str. 219-229. [COBISS.SI-ID 28465925]
- GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Synthesis of spiro[bicyclo[2.2.1]heptane-2,2'-furan]-3-amines via stereoselective cycloadditions of trimethylenemethane to (1S,3EZ,4R)-3-arylimino-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ones. *Tetrahedron: asymmetry*, ISSN 0957-4166. [Print ed.], 2007, vol. 18, no. 19, str. 2365-2376. [COBISS.SI-ID 29014789]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MODERNE NMR METODE
Course Title:	MODERN NMR METHODS

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: K2I10

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

Nosilec predmeta / Lecturer: prof. dr. Janez Plavec / Dr. Janez Plavec, Full 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):**
Uvod. Osnove NMR eksperimenta, kemijski premik, sklopitve, integrali, običajno merjeni nuklidi, klasične in pulzne tehnike. **Magnetne lastnosti jeder.** Jedro v magnetnem polju, Energetski nivoji, relaksacijski časi, vektorski opis vzorca, laboratorijski in rotirajoč koordinatni sistem, pulz. **Sklopitvena konstanta.** Spektri prvega in drugega reda, kemijska in magnetna ekvivalenca jeder, predznak in velikost sklopitvene konstante, sklopitev preko ene, dveh, treh in več vezi. **Povezava strukture spojine in kemijskih premikov.** Vplivi na kemijske premike ^{1}H in ^{13}C, programska oprema za napoved kemijskih premikov. **Merjenje NMR spektra.** Magnet, CW in pulzni	Basics of NMR experiment, chemical shift, coupling, integral, frequently measured nuclei, classical pulse sequences. Magnetic properties of nuclei. A nucleus in magnetic field, energy levels, relaxation times, vector description of a sample, laboratory and rotating frame coordinate system, pulse. Coupling constant. First and higher order spectra, chemical and magnetic equivalence, sign and magnitude of coupling constant, one-, two, or more-bond coupling. Relation between structure and chemical shifts. Chemical shift dependence on molecular structure, NMR spectral prediction software. Acquisition of NMR spectra. Magnet, Continuous wave and pulse mode, data acquisition, FID, Fourier transformation,

način, zajemanje podatkov, FID, Fouriejeva transformacija, matematične manipulacije FID, **Študij dinamičnih procesov z NMR.** **Moderne pulzne NMR tehnike.** Manipulacija magnetizacije, spin-echo pulzna sekvenca in njene posledice; prenos polarizacije in editiranje spektrov; nuklearni Overhauserjev efekt; uvod v dvo- in večdimenzionalne NMR eksperimente. **Dvodimenzionalne NMR tehnike**. Pregled principov in uporabe dvodimenzionalnih NMR metod pri določanju kemijske strukture in konformacije molekul v raztopini COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC, NOESY. **Vaje** Priprava vzorca in inštrumenta; 1D eksperimenti (^{1}H, ^{13}C, X); 2D eksperimenti (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).	mathematical manipulation of FID. Study of Dynamic processes by NMR. Modern pulse NMR. Manipulation of magnetization, spin-echo pulse sequence, polarization transfer and spectral editing, nuclear Overhouser effect, introduction to two- and more-dimensional NMR experiments. Two-dimensional NMR techniques. Overview of principles and application of 2D NMR methods in structure elucidation and conformational studieS in solution, COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC, NOESY. Practical spectroscopy: sample preparation, basic instrumental procedures, one-dimensional experiments ($_{1}$H, $_{13}$C, X), two-dimensional experiments (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).

Temeljna literatura in viri / Readings:

1. James Keeler Understanding NMR Spectroscopy, ISBN: 0-470-01787-2, oktober 2005
2. Thomas C. Pochapsky & Susan Sondej Pochapsky, NMR for Physical and Biological Scientists, ISBN: 0 8153 4103 2, 2007
3. Neil E. Jacobsen, NMR Spectroscopy Explained, ISBN: 978-0-471-73096-5, John Wiley & Sons, 2007

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Študent pridobi znanja, ki so potrebna za razumevanje modernih NMR tehnik, načrtovanje in izvedbo eksperimentov njihovo uporabo in interpretacijo rezultatov. *Kompetence:* Pridobljeno znanje študentu omogoča samostojno načrtovanje NMR eksperimentov, njihovo praktično izvedbo in interpretacijo rezultatov.	**Objectives:** To teach students theory and practice of modern NMR methods necessary to understand modern MMR techniques, planning and performing experiments and interpretation of the results. **Competences:** Ability to design, perform, and interpret NMR experiments for the determination of structure and conformation of compounds in solution.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Poznavanje principov in praktične izvedbe modernih NMR eksperimentov za določanje strukture in konformacije spojin v raztopini.	<u>Knowledge and Comprehension</u> Understanding the basic principles and practical knowledge about NMR experiments.

Uporaba Študent uporabi pridobljeno znanje NMR spektroskopskih tehnik pri reševanju raziskovalnih problemov.	Application Student utilizes the acquired knowledge in solving research problems
Refleksija Zavedanje, da z NMR tehnikami pridobimo pomembne informacije o strukturi in konformaciji molekul v raztopini in da so NMR tehnike najpomembnejša analitska metoda v organski kemiji.	Analysis Student applies the acquired NMR spectroscopy knowledge and skills in solving research problems.
Prenosljive spretnosti Pri predmetu se študenti se izurijo v načrtovanju in izvedbi eksperimentov ter kritični interpretaciji rezultatov.	Skill-transference Ability Student is trained in planning and utilization of NMR spectroscopic methods, analytical thinking and using literature sources.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja in vaje	Lectures and practical laboratory work

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Ustni izpit in praktični preskus. 10 (odlično), 9 in 8 (prav dobro), 7 (dobro), 6 (zadostno), 5-1 (nezadostno)		

Reference nosilca / Lecturer's references:

() M.L. Greco, A. Kotar, R. Rigo, C. Cristofari, J. Plavec and C. Sissi, Nucleic Acids Res. 2017, 45, 10132.
() V. Kocman, J. Plavec, Nat. Commun. 2017, 8; 15355.
() M. Gajarský, M. Lenarčič Živković, P. Stadlbauer, B. Pagano, R. Fiala, J. Amato, L. Tomáška, J. Šponer, J. Plavec, L. Trantírek, J. Am. Chem. Soc. 2017, 139, 3591.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MOLEKULSKO MODELIRANJE
Course Title:	MOLECULAR MODELLING

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: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE221

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

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee / dr. Barbara Hribar Lee, Full Professor
doc. dr. Črtomir Podlipnik / dr. Črtomir Podlipnik, 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):
Osnovni pojmi v molekulskem modeliranju. Zapis molekul. Molekulska grafika. Molekulske površine. Kvantnomehanski modeli. Schrödingerjeva enačba. Večelektronski sistemi. Variacijska metoda – Hartree-Fockov sistem enačb. Roothaan-Hallove in Pople-Nesbetove enačbe. Bazne funkcije in bazni seti. Korelacijska energija – konfiguracija interakcij in Møller-Plessetova perturbacijska teorija. Semiempirične metode. Teorija gostotnega funkcionala. Molekulske lastnosti, dobljene iz valovne funkcije. Mehanski modeli – empirična polja sil. Vezne interakcije. Nevezne interakcije. Reducirana	Useful concepts in molecular modelling. Molecular file formats. Molecular graphics. Molecular surfaces. Quantum mechanical models. Schrödinger equation. Polyelectronic systems. Variation method - Hartree-Fock equations. Roothaan-Hall and Pople-Nesbet equations. Basis functions and basis sets. Correlation energy – configuration interaction and Møller – Plesset perturbation theory. Semi-empirical methods. Density functional theory. Calculating molecular properties from the wave function. Molecular mechanics – empirical force field models. Bonded interactions. Non-bonded interactions. Reduced representation. Force

reprezentacija. Modeli za opis vode. Ovrednotenje rezultatov molekulske mehanike. Energijska minimizacija. Računalniške simulacije. Zasnova računalniških simulacij. Računalniška simulacija Monte Carlo. Računalniška simulacija molekulske dinamike. Simulirano ohlajanje. Konformacijska analiza. Vaje: uporaba različnih metod molekulskega modeliranja na praktičnih primerih.	field models for water. Calculating systems properties from molecular mechanics. Energy minimisation. Computer simulations. Basic elements of computer simulations. Monte Carlo computer simulation. Molecular dynamics computer simulation. Simulated annealing. Conformational analysis. Lab work: applying the methods of molecular modelling to practical examples.

Temeljna literatura in viri / Readings:

- B. Hribar-Lee, Č. Podlipnik, Molekulsko modeliranje, skripta za predavanja in vaje, interno gradivo.
- A. R. Leach, Molecular Modelling, Principles and Applications, Addison Wesley Longman, London, 1998.

Dodatna literatura:

- F. Jensen, Introduction to Computational Chemistry, Wiley, Hoboken, 2007.
- A. Szabo, N. S. Ostlund, Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, Dover, New York, 1996. (10%)

Cilji in kompetence:	**Objectives and Competences:**
Cilji modeliranja: poznavanje elektronske strukture in geometrije molekul (iz osnovnih podatkov), napoved lastnosti molekul in njihova povezava s strukturo, podobnost molekul, možnost načrtovanja molekul z vnaprej določenimi želenimi lastnostmi. *Kompetence:* razumevanje in obvladovanje vloge računalniške grafike pri molekulskem modeliranju. Pregled najbolj znanih računalniških programov za uporabo pri modeliranju (Gaussian, Spartan, HyperChem ...), prikaz praktičnega dela na osebnem računalniku, delovni postaji in velikem računalniku (preko računalniške mreže). Sistematični pregled celotne snovi.	Objectives: The knowledge (prediction) of molecular geometry and molecular electronic structure. The use of molecular modeling and quantum mechanical methods for prediction of molecular properties. Qualitative and quantitative structure-property relationships. Structure based design of molecules with certain properties. Competences: Overview of well-known programs for molecular modeling and quantum chemical computations as such as Gaussian, Spartan, HyperChem, Schrodinger Suite with hands on sessions on personal comuterm working station and big cluster (using web interface).
Predvideni študijski rezultati:	**Intended Learning Outcomes:**

Znanje in razumevanje Predmet je namenjen nadgradnji znanja kvantne kemije in njeni praktični uporabi. Študente seznani s pojmom molekulskega modeliranja, ki je že dalj časa močno orodje za pomoč eksperimentalistom, saj omogoča vpogled na nekatera eksperimentom nedostopna področja znanosti. Ob koncu so sposobni formulirati problem, izbrati primerno metodo modeliranja in kritično ovrednotiti dobljene rezultate. Pomembno je potem tudi iskanje korespondence med dobljenimi teoretičnimi in v literaturi poiskanimi rezultati.	Knowledge and Comprehension This course is designed to upgrade the knowledge of quantum chemistry and its practical application. During this course the students will be introduced with molecular modeling methods and principles. Molecular modeling became an excellent toll that serve as support to experimentalist for better understanding fundamental and applicative science. At the end of the course students will be able to formulate problem, to select and to set up a proper molecular modeling method, and also to evaluate obtained results critically. They will be also able to compare the experimental data either from literature and/or laboratory with the data resulted from computional chemistry approach.
Uporaba Slušatelj je sposoben uporabiti znanje kvantne kemije za modeliranje danega kemijskega ali biokemijskega problema, komercialne računalniške programske sisteme s tega področja mu ni več potrebno uporabljati kot "black box", zaradi česar lahko tudi mnogo bolj kompetentno razlaga dobljene rezultate.	Application The student is able to use quantum chemistry knowledge for modeling of certain chemistry orbiochemistry problem. The background that the student obtains in the course transforms her/him into an advanced user of computational chemistry software. They are able to competently interpret computational chemistry results.
Refleksija Študent si pridobi občutek, da se lahko v primeru nepremostljivih eksperimentalnih težav še vedno zateče k računu, kjer so problemi drugačni in navadno drugje, kar pogosto privede do zadovoljive razjasnitve problema.	Analysis The information from the computational experiment are often complementary than those obtained from laboratory experiment. The proper combination of laboratory and computational work often leads to more relevant description of the problem.
Prenosljive spretnosti Pri predmetu se študenti naučijo prepoznavati problem, ga prevesti v matematično obliko, rešiti in na koncu interpretirati rezultate. Poseben poudarek je na kritičnem ovrednotenju dobljenih rezultatov. Naučijo se uporabe domače in tuje literature ter podajanja zaključenega dela v pisni obliki.	Skill-transference Ability In this course the students are able to recognize a problem, to transform it to mathematical form, to solve the problem and at the end to interpret results. The critical evaluation of the results is one of the most important skills that students learn during the course. At the end of the course the students learn how to write a scientific report and to perform scientific presentation.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**

- Predavanja - Seminar (računske naloge iz predelane snovi) - Praktične vaje na računalniku	- Lectures - Seminars - Laboratory Lessons (Using computer)

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit	**50 %**	Written exam
Seminarska naloga	**50 %**	Seminar
Ocene: 6 – 10 (pozitivno)		

Reference nosilca / Lecturer's references:

prof. dr. Barbara Hribar Lee:
- M. Luksic, T. Urbic, B. Hribar-Lee, K. A. Dill, Simple Model of Hydrophobic Hydration, J. Phys. Chem. B, 2012, 116 (21), 6177– 6186.
- B. Hribar-Lee, K. A. Dill, V. Vlachy, Receptacle Model of Salting- In by Tetramethylammonium Ions, J. Phys. Chem. B, 2010, 114 (46), pp 15085–15091.
- K. A. Dill, T. M. Truskett, V. Vlachy, B. Hribar-Lee, Modeling water, the hydrophobic effect, and ion solvation, Annu Rev Biophys Biomol Struct, 2005, 34, 173-199.

doc. dr. Črtomir Podlipnik:
- SKRT, Mihaela, BENEDIK, Evgen, PODLIPNIK, Črtomir, POKLAR ULRIH, Nataša. Interactions of different polyphenols with bovine serum albumin using fluorescence quenching and molecular docking. *Food chem.*. [Print ed.], 2012, vol. 135, str. 2418-2424, doi: 10.1016/j.foodchem.2012.06.114. [COBISS.SI-ID 4113784]
- MARUŠIČ, Jaka, PODLIPNIK, Črtomir, JEVŠEVAR, Simona, KUZMAN, Drago, VESNAVER, Gorazd, LAH, Jurij. Recognition of human tumor necrosis factor [alpha] (TNF-[alpha]) by therapeutic antibody fragment : energetics and structural features. *J Biol Chem*, 2012, vol. 287, no. 11, str. 8613-8620, doi: 10.1074/jbc.M111.318451. [COBISS.SI-ID 35833349]
- PODLIPNIK, Črtomir, TUTINO, Federico, BERNARDI, Anna, SENECI, Pierfausto. DFG-in and DFG-out homology models of TrkB kinase receptor : induced-fit and ensemble docking. *J. mol. graph. model.*. [Print ed.], 2010, vol. 29, no. 3, str. 309-320, doi: 10.1016/j.jmgm.2010.09.008. [COBISS.SI-ID 34621701]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	NAPREDNE INŠTRUMENTALNE ANALIZNE TEHNIKE
Course Title:	ADVANCED METHODS OF INSTRUMENTAL ANALYSIS

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

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE222

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	15	15 LV	/	/	75	5

Nosilec predmeta / Lecturer: prof. dr. Helena Prosen / Dr. Helena Prosen, Full Professor
prof. dr. Matevž Pompe / Dr. Matevž Pompe, Full 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):
Kemometrični pristopi v instrumentalni analizi, npr. ANOVA, PCA. Kvantitativna IR spektroskopija, ATR, DR. Ramanska spektroskopija. Sodobne eno in večdimenzionalne kromatografske separacije. Kapilarna elektroforeza. Sklopitve kromatografskih in spektroskopskih tehnik. Pregled sodobne molekulske masne spektrometrije in sklopljenih tehnik. Ionizacijske tehnike, masni analizatorji, tandemska masna spektrometrija. Aplikacije	Chemometric approaches in instrumental analysis, e.g. ANOVA, PCA. Quantitative IR spectroscopy, ATR, DR. Raman spectroscopy. Modern one- and multidimensional chromatographic separations. Capillary electrophoresis. Hyphenations of chromatographic and spectroscopic techniques. Overview of modern molecular mass spectrometry and hyphenated techniques. Ionization techniques, mass analyzers, tandem mass spectrometry. Applications of MS.

MS. Elementna masna spektrometrija in sklopljene tehnike. Osnove tehnik za karakterizacijo površin: elektronska spektroskopija in elektronska mikroskopija. Analitika ultrasledov: nevtronska aktivacijska analiza. Avtomatizirana analiza, robotizirana analiza, miniaturni sistemi. Senzorji: elektrokemijski, optični, imunski, drugi tipi. Seminarji in vaje projektnega tipa: teoretična obdelava literaturnih rešitev za praktične analizne probleme z uporabo analiznih tehnik, predstavljenih na predavanjih. Demonstracijske vaje.	Elemental mass spectrometry and hyphenated techniques. Basics of techniques for surface characterization: electron spectroscopy and electron microscopy. Analytics of ultra-trace components: neutron activation analysis. Automated analysis, robotic analysis, miniaturized systems. Sensors: electrochemical, optical, immunosensors, other. Seminars and laboratory work projects: theoretical discussion of literature solutions for practical analytical problems by the use of discussed analytical techniques. Demonstrative laboratory work.

Temeljna literatura in viri / Readings:

- Analytical Chemistry A Modern Approach to Analytical Science, Ed. by R. J.- Mermet, M. Otto, M. Valcarcel, Founding Editors: R. Kellner, H.M. Widmer, Wiley - VCH, Weinheim, 2004, izbrana poglavja, ca. 300 strani

<u>Dodatna literatura:</u>

- F. Rouessac, A. Rouessac, Chemical Analysis, Modern Instrumentration Methods and Techniques, J. Wiley & Sons, Ltd, Chichester, 2000.
- pregledni znanstveni članki iz posameznih področij / scientific review articles from different fields

Cilji in kompetence:	**Objectives and Competences:**
Študenti se seznanijo s kemometričnimi in numeričnimi pristopi v analizni praksi, spoznajo napredne metode za analizo in kontrolo bioloških učinkovin in snovi ter karakterizacijo in analizo anorganskih in organskih materialov. Seznanijo se z analitiko sledov, ugotavljanjem kemijskih zvrsti in avtomatizacijo analiznih metod in postopkov.	Students are informed of chemometric and numerical approaches in the analytics; they learn about the advanced analytical methods for biological active components control and for characterization and analysis of inorganic and organic materials. They are introduced to trace analysis, chemical speciation and automation of analytical methods and procedures.
Predvideni študijski rezultati:	**Intended Learning Outcomes:**

Znanje in razumevanje Obvladovanje kemometričnih pristopov, numeričnih postopkov optimizacije, modeliranja in statistične obravnave podatkov. Razumevanje principov, delovanja in omejitev posameznih analiznih tehnik za analizo materialov in bioloških sistemov ter poznavanje in razumevanje pristopov za avtomatizacijo analiznih metod.	Knowledge and Comprehension Mastering of chemometric approaches, numerical optimization methods, modelling and statistical data evaluation. Understanding of the concepts, working principles and limitations of certain analytical techniques for the analysis of materials and biological systems; knowledge and understanding of the approaches to analytical method automation.
Uporaba Študent pridobi znanja za uporabo na področju kemijskih raziskav ter na področju raziskav materialov in bioloških snovi.	Application Student acquires practical knowledge to use in chemical research and research of materials and biological samples.
Refleksija Poveže konkretno uporabo določene kemijsko-fizikalne zakonitosti z rezultati, ki jih pridobi z meritvemi.	Analysis Student connects the application of a certain physico-chemical principle with the results obtained by the measurement.
Prenosljive spretnosti Osvoji metodologijo in raziskovalne pristope, obvlada problemsko orientirane raziskave, zna uporabljati strokovno in znanstveno literaturo in obvlada veščine poročanja in obravnave podatkov.	Skill-transference Ability Student masters the methodology and research approaches, as well as problem-oriented research; knows how to use professional and scientific literature; masters the skill of data evaluation and presentation.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja in seminarska dela iz aktualne tematike, demonstracijske vaje	Lectures, seminar coursework on realistic problems, demonstrative laboratory work

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni in ustni izpit: ocene od 6-10 (poz.) oz. 1-5 (neg.).	**60 %**	Written and oral exam: grades 6-10 (pass) or 1-5 (fail).
Seminarska naloga.	**30 %**	Seminar coursework.
Laboratorijske vaje.	**10 %**	Laboratory work.
Opravljene vaje in seminarska naloga so pogoj za pristop k izpitu.		Finished laboratory and seminar work are prerequisites for the exam.

Reference nosilca / Lecturer's references:

- A. Ćirić, **H. Prosen**, M. Jelikić Stankov, P. Đurđević. Evaluation of matrix effect in determination of some bioflavonoids in food samples by LC-MS/MS method. *Talanta* 2012, 99, 780-790.
- **H. Prosen**, M. Kokalj, D. Janeš, S. Kreft. Comparison of isolation methods for the determination of buckwheat volatile compounds. *Food Chem.* 2010, 121, 298-306.

- I. Kralj Cigić, **H. Prosen**. An overview of conventional and emerging analytical methods for the determination of mycotoxins. *Int. J. Mol. Sci.* 2009, 10, 62-115.
- S. Kose, S. Koral, B. Tufan, **M. Pompe**, A. Ščavničar, D. Kočar. Biogenic amine contents of commercially processed traditional fish products originating from European countries and Turkey. European Food Research and Technology. A, Zeitschrift für Lebensmittel-Untersuchung und -Forschung. 2012, 235, 669-683.
- G. Arh, L. Klasinc, M. Veber, **M. Pompe**. Calibration of mass selective detector in non-target analysis of volatile organic compounds in the air. J. chromatogr. A 2011, 1218, 1538-1543.
- J. Cerar, **M. Pompe**, M. Guček, J. Cerkovnik, J. Škerjanc. Analysis of sample of highly water-soluble T[sub]-symmetric fullerenehexamalonic acid C[sub](66)(COOH)[sub](12) by ion-chromatography and capillary electrophoresis. J. chromatogr. A 2007, 1169, 86-94.

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: izr. 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.

atmosferi in vakuumu.	Acquire knowledge of the principles of catalytic processes and understanding the role of metals 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 chemistr y 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

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, 2nd Cycle	/	1st	2nd

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: izr. 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:	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. 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.**	1. Mechanism of a chemical reaction: definitions, elementary and stepwise reactions, bond making and bond breaking, molecularity, formulating mechanisms. 2. Kinetics and thermodynamics of organic reactions: Equilibrium and rate constants, acids, bases, pKa, pH, kinetic order, application of kinetic data in formulating the mechanism, the dependence of rate of reaction on temperature, primary kinetic isotopic effect. 3. 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 (□) in ro (□)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:	**Intended Learning Outcomes:**
Znanje in razumevanje Poznavanje poteka osnovnih organskih reakcij in metod za študij oziroma dokazovanje reakcijskih mehanizmov. Razumevanje in poznavanje vplivov na potek kemijskih reakcij.	Knowledge and Comprehension Understanding the principles and methods of postulating the reaction mechanism of an organic reaction. Understanding the influence of different parameters on reaction course.
Uporaba Razvita sposobnost študenta, da pridobljeno znanje uporabi za raziskavo mehanizma neznane reakcije.	Application Student will be able to apply the acquired knowledge in reaction mechanism investigation.
Refleksija 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.	Analysis Being aware that chemical reactions never follow exclusively one elementary mechanism and that for complete analysis every reaction requires thorough investigation.
Prenosljive spretnosti Pri predmetu se študenti z reševanjem znanih in neznanih problemov izurijo v uporabi znanja, analitičnega mišljenja in uporabe literaturnih virov.	Skill-transference Ability Using known and unknown examples the student is trained in utilization of knowledge, analytical thinking and using literature sources.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja in vaje.	Lectures and practical laboratory work.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit.		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]

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	PODJETNIŠTVO
Course Title:	ENTREPRENEURSHIP

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	/	2.	4.
USP Chemistry, 2nd Cycle	/	2nd	4th

Vrsta predmeta / Course Type: izbirni splošni / Elective General

Univerzitetna koda predmeta / University Course Code: SI102

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

Nosilec predmeta / Lecturer: prof. dr. Mateja Drnovšek / Dr. Mateja Drnovšek, Full 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):**
Študenti bodo v okviru predmeta spoznali: - pomen podjetništva v gospodarstvu in temeljne pojme podjetništva - prepoznavanje poslovnih priložnosti - dinamična podjetja in razvoj novih izdelkov in storitev v obdobju globalizacije - pet korakov razvoja novih izdelkov in storitev – opazovanje, brainstorming, hitro prototipiranje, izboljšanje prototipov in implementacija rešitve. - dizajnerski način razmišljanja – tehnični, poslovni, človeški vidik - kreativnost in inovativnost v poslovnem in privatnem življenju - tehnike spodbujanja kreativnosti - praktična aplikacija metode razvoja novih	Students will learn: – Entrepreneurship and its role in the socio-economic development – Developing entrepreneurial opportunities – Dynamic companies and development of new products in a globalized world – Five steps of product development process: observation, brainstorming, rapid prototyping, testing and refinement and implementation – Design thinking – desirability, feasibility, viability of new solutions – Creativity and innovativeness in personal and business life – Techniques of developing creativity

izdelkov in dizajnerskega procesa - okolje podjetja in njegova analiza - različne oblike družb z oceno njihovih prednosti in slabosti - osnove računovodstva in financiranja - poslovno načrtovanje, vsebino in način izdelave poslovnega načrta - politiko spodbujanja podjetništva države - pomen in vsebino marketinške/prodajne funkcije v podjetju - metode raziskovanja trga, porabnikov, konkurence - temeljna znanja iz projektnega menedžmenta - poslovno komunikacijo - primere uspešnih slovenskih izdelkov, podjetij, podjetnikov	– Practical application of new product development methodologies and design thinking – Business environment and it's analysis – Different form of enterprise and their differences – Basics of accounting and financing – Business planning, contents and the development of a business plan – Governmental policies on supporting entrepreneurship – Role definition of marketing and sales – Methods of customer, competition and market analysis – Basic project management skills – Business communication – Examples of successful Slovenian products, companies, entrepreneurs

Temeljna literatura in viri / Readings:

- Vahčič, A., Prodan, I., in ostali: D.SCHOOL RAZVOJ NOVIH PRODUKTOV IN STORITEV - Od interdisciplinarnosti in dizajnerskega način razmišljanja do uspeha na trgu, 2008
- Kelley, T.: The Ten Faces of Innovation: IDEO's Strategies for Defeating the Devil's Advocate and Driving Creativity Throughout Your Organization
- Kelley, T. et al: The Art of Innovation: Lessons in Crativity from IDEO, America's Leading Design Firm
- dodatna aktualna gradiva, objavljena na spletni strani predmeta

Dopolnilna literatura:

- Antončič,B., Hisrich, R., Petrin,T.,Vahčič,A.,Podjetništvo, Založba GV, Ljubljana, 2002, 485 str.

Cilji in kompetence:

Cilj predmeta je študentom razviti sposobnost timskega dela, prevzemanja odgovornosti in samoiniciativnega delovanja pri reševanju človeških, tehničnih in ekonomskih problemov povezanih z razvojem novih produktov in storitev. Študentje z uporabo dizajnerskega pristopa in hitrega prototipiranja izdelajo delujoč prototip rešitve problema. Poleg tega predmet razvija sposobnost dizajnerskega in holističnega razmišljanja kot sodobne tehnike za reševanje problemov. Študentje osvojijo tudi zmožnosti za presojo poslovanja v podjetjih, sposobnosti za presojo poslovnih priložnosti in pridobijo kompetence za samostojno vodenje.

Objectives and Competences:

The aim of the course is to develop the ability of teamwork, responsibility, taking the initiative, and the ability to solve any societal, technical or business problem associated with developing new products and services. Students will be using Design Thinking and rapid prototyping to produce a working prototype of a solution to a given problem. In addition, the subject develops design thinking and holistic thinking as modern techniques for problem solving. Students acquire the ability to assess the operation of enterprises, the ability to assess business opportunities and gain skills for managing a small business.

Študentje si pri predmetu pridobijo naslednje **specifične kompetence**: - prepoznavanje in izkoriščanje podjetniške priložnosti - metode raziskav trga, kupcev, konkurence - kreativno in inovativno reševanje problemov - uporaba sodobnih multimedijskih in telekomunikacijskih orodij - funkcionalno poslovno pismenost in osnove poslovnih predstavitev - usposobljenost za vodenje projektov, prenos znanja v prakso, analizo poslovanja podjetij	Students obtain the following specific competencies: - Identification and exploitation of business opportunities - Methods of market research (including customers and competition) - Creative and innovative problem solving - The use of modern media and telecommunication tools - Functional business literacy and basics of business presentations - Ability to manage projects, transfer of knowledge into practice, analysis of businesses

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Študent bo spoznal in razumel: - pojme s področja podjetništva in gospodarstva, organizacije dela, vodenja projektov, marketinga - osnovne zakonitosti kreativnega razvoja novih izdelkov in storitev ter podjetniške dejavnosti s poudarkom na primerih iz prakse kakor tudi iz študentovih življenjskih potreb ter izkušenj	Knowledge and Comprehension The student will recognise and understand: - Concepts in the field of entrepreneurship and economy as a whole, management, project management, marketing - The basic principles of creative development of new products and services, and entrepreneurial activities with an emphasis on case studies as well as from the student's needs and life experiences
Uporaba Predmet je usmerjen v praktično uporabo najnaprednejših metod razvoja novih izdelkov in storitev. Skozi dizajnerski način razmišljanja in s pomočjo d.school metodologije študent reši konkreten poslovni ali življenjski problem in osvoji znanje, ki ga lahko replicira v profesionalnem in osebnem življenju. Prepoznavanje podjetniških priložnosti, analiza podatkov in informacij za sprejemanje poslovnih odločitev, izdelava prototipov, antropološke in etnografske metode spremljanja potrošnikov, izpeljava rešitve problema. Dokumentacija procesa z multimedijskimi metodami, samostojna priprava finančnih in poslovnih analiz (trženjskih, prodajnih ipd).	Application The course is focused on the practical application of advanced methods of developing new products and services. Through design thinking methodology students solve a specific business or societal problem and acquire knowledge that can be replicated in professional and personal life. Identifying business opportunities, analysis of data and information for business decision-making, prototyping, anthropological and ethnographic methods of customer analysis, implementing solutions to a specific problem. The documentation of the process with multimedia, independent preparation of financial and business analyses (marketing, sales, etc.).
Refleksija Študent bo interpretiral ter pred kolegi analiziral lastno razumevanje vsebine aktualnih člankov in razpoznavanja trendov. V skupinskem delu študentje analizirajo delo	Analysis The student will interpret and in front of colleagues analyse her understanding of articles on current topics and show recognition of trends. In group work, students analyse their

svoje in ostalih skupin in podajajo konstruktivno kritiko.	own work and work of other groups and give constructive feedback.
Prenosljive spretnosti Pri predmetu bo študent pridobil sposobnosti razumevanja podjetništva, razpoznavanja poslovnih priložnosti, analize trgov, potrošnikov, konkurence. Uporaba replikativne metodologije reševanja problemov in udejanjanja poslovnih priložnosti. Poslovna komunikacija. Pridobljene spretnosti bodo študentje znali uporabljati v osebnem in profesionalnem življenju, v delu v gospodarstvu ali javnem sektorju. Sposobnost `gradnje` boljših modelov namesto izbiranja med obstoječimi modeli.	Skill-transference Ability In this course the student will acquire the ability to understand entrepreneurship, identify business opportunities, analyse markets, consumers, competition. Use of a replicative methodology of problem solving and realizing business opportunities. Business communication. Students will be able to use the acquired skills in their personal and professional life, either in business or in the public sector. The ability to develop better models instead of selecting between existing models.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja s pomočjo različnih AV sredstev. Študentom podamo uvod v obravnavano snov, jih napotimo na obravnavo člankov v medijih, na spletnih straneh, na obravnavo primerov iz vsakdanje prakse – tudi s pomočjo strokovnjakov iz prakse. Delo na konkretnem projektu, aktualnem problemu. Predstavitve sprotnega dela, poročilo in komentarji s strani mentorjev in študentov. Uporaba multimedijske tehnologije za spremljanje napredka, Internet, video Aktivno mentorstvo s strani pedagogov, asistentov, praktikov - podjetnikov Terensko delo – analiza trga, potrošnikov, testiranje prototipov, uporaba rešitve problema, praktične vaje d.school metodologije	Lectures using audio-visual technology. We give students an introduction to specific topics, assign them to read articles in the media, on websites. Students will deal with cases from everyday practice - with the help of experts from practice. Work on a specific project in form of a real business or societal problem. Ongoing work will be regularly presented and comments will be given by tutors and students. The use of multimedia (Internet, video, etc.) for monitoring progress. Active mentoring will be available by teachers, assistants, practitioners – entrepreneurs. Fieldwork - market analysis, prototype testing, implementing the solution, practical exercises of the design thinking methodology

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Redna poročila o napredku	**20**	Regular progress reports
Končno poročilo in predstavitev o rešitvi problema	**40**	Final report and presentation on the solution of the problem
Domače naloge, sodelovanje na srečanjih	**20**	Homeworks and active participation in sessions
Izpit pisni in/ali ustni. Ocene: 6-10 pozitivno	**20**	Written and / or oral exam. Grades 6-10.

Reference nosilca / Lecturer's references:

- Ahlin, Branka, **Drnovšek, Mateja**, Hisrich, Robert D. (2014). Entrepreneurs creativity and firm innovation : the moderating role of entrepreneurial self-efficacy. Small business economics,
- Slavec, A., **Drnovšek, M** (2012). A perspective on scale development in entrepreneurship research. Economic and Business Review, 14(1), pp. 39-62
- Ahlin, B., **Drnovšek, M.**, Hisrich, R.D. (2012). Exploring moderating effects of proactivity on the relationship between market information and innovation performance. Economic and Business Review, 14(2), pp. 121-146.
- **Drnovšek, M**., Örtqvist, D., Wincent, J. (2010). The effectiveness of coping strategies used by entrepreneurs and their impact on personal well-being and venture performance. Zb. rad. Ekon. fak. Rij., 28(2), pp. 193-220.
- Prodan, I., **Drnovšek, M.** (2010). Conceptualizing academic- entrepreneurial intentions: an empirical test. Technovation, 30 (5/6), pp. 332-347
- **Drnovšek, M.**., Wincent, J., Cardon, M. (2010). Entrepreneurial self-efficacy and business start-up: developing a multi-dimensional definition. International Journal of Entrepreneurial Behavior and Research, 14 (4), pp. 329-348.
- Cardon, M., Wincent, J., Singh, J. **Drnovšek, M.** (2009). The nature and experience of entrepreneurial passion. Academy of. Management Review, 34 (3), pp. 511-532.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	RAZISKOVALNO DELO
Course Title:	RESEARCH WORK

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

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE215

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
/	**/**	**/**	**/**	**300**	**/**	**20**

Nosilec predmeta / Lecturer: /

Jeziki / Languages: **Predavanja / Lectures:** **/**
Vaje / Tutorial: **/**

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):
Raziskovalno delo se opravlja na področju kemije. Vsebina in naslov se določata v soglasju z izbranim mentorjem – nosilcem ene izmed vsebin v programu.	Research work must be carried out in the area of chemistry; Student may choose specific area and mentor; Contents of research work are agreed upon with the mentor, who must be a lecturer of at least one of topics of the programme.

Temeljna literatura in viri / Readings:

- Knjige in članki, ki so povezani z vsebino raziskovalnega dela.

- Textbooks and journal articles from the field of the research work

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta je, da študenti s pomočjo laboratorijskega praktičnega dela uporabijo usvojena teoretična znanja in v praksi izvedejo raziskovalno nalogo. Pri tem uporabijo oziroma usvojijo potrebne instrumentalne in druge karakterizacijske tehnike, dobljene rezultate pa kritično ovrednotijo. Študentje pri predmetu pridobijo naslednje specifične *kompetence:* - sposobnost uporabe pridobljenih znanj na specifičnem raziskvalnem področju kemika; - sposobnost samostojnega opravljanja raziskovalnega in razvojnega dela.	Contact with experimental techniques of chemistry; Applying theoretical knowledge in practice; To get the experience in using different engineering tools and devices for process control and for product synthesis; To get the experience in using supporting instrumental and analytical techniques indispensable to collect experimental data; To get the experience in using different software packages for quantitative data analysis in accordance with theoretical predictions; Critical evaluation and presentation of the results in a scientific report. Subject specific competences are the use of theoretical knowledge in a specific area of chemical engineering and independent research and development work.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Med opravljanjem raziskovalnega dela bo študent pridobil: • sposobnosti formuliranja problema, • sposobnosti samostojnega iskanja ustrezne literature, • sposobnosti obravnavanja problema v praksi, • sposobnosti iskanja kvantitativnih rešitev in utemeljevanja ustreznosti rešitev, sposobnosti predstavitve rezultatov svojega dela.	Knowledge and Comprehension Ability of problem formulating; Ability of literature researching; Ability of problem managing in practice; Ability of quantitative problem solving and argumentation of the solution; Ability to present research results.
Uporaba Znanje in pridobljene veščine bo študent lahko uporabil pri opravljanju poklica in opravljanju magistrkega dela.	Application Acquired knowledge is necessary for Master's thesis work and for professional work.
Refleksija Povezovanje vseh pridobljenih teoretičnih znanj z reševanjem problemov na področju kemije ter kritični pogled na uporabnost teh znanj.	Analysis Integration of knowledge from different topics of chemistry and supporting sciences; Development of a critical view on the knowledge applicability.

Prenosljive spretnosti Pri delu bo študent pridobil znanja o metodah reševanja kompleksnih problemov, o načinu prezentacije teh znanj v pisani in govorjeni obliki povezani z ostalimi metodami posredovanja raziskav, ugotovitev itd.	Skill-transference Ability Ability of solving complex problems using different methods and skills; Ability of presenting the research work in a written and oral form.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Individualno delo mentorja in samostojno študijsko in raziskovalno delo.	Independent research work supervised by the mentor.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Oddano poročilo o delu in ustna predstavitev poročila na seminarju. Oboje oceni mentor. Ocena: opravil/ni opravil.		pass/fail

Reference nosilca / Lecturer's references:

/

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	SODOBNI ANORGANSKI MATERIALI IN KATALIZATORJI
Course Title:	MODERN INORGANIC MATERIALS AND CATALYSTS

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, 2nd Cycle	**/**	**1st**	**2nd**

Vrsta predmeta / Course Type: obvezni/ Mandatory

Univerzitetna koda predmeta / University Course Code: K2I03

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

Nosilec predmeta / Lecturer: doc. dr. Romana Cerc Korošec / Dr. Romana Cerc Korošec, Assistant Professor
prof. dr. Anton Meden / Dr. Anton Meden, Full 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):
Kemija materialov: - uvod: različni tipi materialov in njihova uporaba; - vplivi kemijske sestave, molekularne in kristalne (ali amorfne) strukture ter mikrostrukture materialov na njihovo funkcijo, polimorfizem; - primeri različnih oblik materialov: monoliti, volumenski materiali, monodisperzni delci, tanki filmi, nano delci; - kemijske osnove in pregled nekaterih postopkov priprave različnih materialov - na primer: reakcije v trdnem, hidrotermalna sinteza, sol-gel metoda, sinteza z uporabo	**Materials chemistry:** - introduction: different types of materials and their application; - the influence of chemical composition, molecular and crystal (or amorphous) structure and microstructure of materials on their function, polymorphism; - examples of different forms of materials: monoliths, bulk materials, monodispersed particles, thin films, nano-particles. - chemical basis and overview of some preparation procedures of different materials – for instance: solid-state reactions, hydrothermal synthesis, sol-gel method, microwave synthesis,

mikrovalov, zgorevalna sinteza, koprecipitacija, priprava monodisperznih delcev, tankih filmov, nanodelcev; - električne, magnetne in optične lastnosti materialov; - osnove heterogene katalize (mehanizem in kinetika reakcij na površini). **Pregled različnih vrst materialov, njihove priprave, strukture in lastnosti:** - molekule v trdninah, samo-urejanje ob kristalizaciji, vpliv oblike molekul na kristalno strukturo; - anorganski, in kovinsko – organski polimeri ter kompoziti; - stekla in keramike, fazni diagrami; - oksidi in nitridi, polprevodniki (dopirani); - kovine in zlitine, napake v kristalih in njihove posledice; - tekoči kristali; **Primeri materialov in njihove uporabe:** - porozni zeolitni in zeolitom podobni katalizatorji; - materiali za shranjevanje in proizvajanje energije – komponente gorivnih celic, baterij in akumulatorjev, trdni ionski prevodniki in fotoelektrokemijske celice; - fotokatalizatorji; - luminiscentni materiali; - kromogeni materiali (elektrokromni, gasokromni, fotokromni, termokromni). - različni nanomateriali. **Vaje:** Skupinska izvedba projekta priprave in karakterizacije materiala po podatkih iz literature.	combustion synthesis, co-precipitation, preparation of uniform particles, thin films, nanoparticles; - electrical, magnetic and optical properties of materials; - the basis of heterogeneous catalysis (mechanism and kinetics of surface reactions). **Overview of different materials, their preparation, structure and properties:** - molecules in solids, self-assembling during crystallization, the influence of molecule`ş shape on crystal structure; - inorganic and metal-organic polymers and composites; - glasses and ceramic materials, phase diagrams; - oxides and nitrides, semiconductors (doped); - metals and alloys, crystal defects and their consequences; - liquid crystals; **Case-studies of materials and their application:** - porous zeolites and zeolite-like catalysts; - materials for energy storage and its production – components of fuel cells, batteries, solid ionic conductors, photoelectrochemical cells, - photocatalysts, - luminescent materials; - chromogenic materials (electrochromic, gasochromic, photochromic, thermochromic) - various nanomaterials. **Practical lab:** Student team performs project from preparation to characterization of materials according to data obtained from the literature.

Temeljna literatura in viri / Readings:

- Introduction to Materials Chemistry, H.A. Allcock, Wiley, 2008, 460 strani (30%).
- Inorganic Materials Chemistry, M.T. Weller, Oxford University Press, 2005, 92 strani (50%).
- Synthesis of Inorganic Materials, U. Schubert and N. Hüsing, Wiley, 2. Izdaja, 2005, 409 strani (25 %).
- The Basis and Application of Heterogeneous Catalysis, M. Bowker, Oxford University Press, 1998, 90 strani (70%).

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Poglobljeno spoznavanje določenih tipov sodobnih anorganskih materialov in katalizatorjev, sinteznih tehnik in raznivrstnih metod za njihovo karakterizacijo. *Kompetence:* Izpeljava celotnega projekta: sinteza in karakterizacije tako katalizatorja kot anorganskega materiala, vključno z literaturnim pregledom in načrtovanjem.	Objectives: Acquiring in-depth knowledge of certain modern inorganic materials, preparation techniques and characterization methods. Competences: Students acquire competences to carry out a project involving synthesis and characterization, both for the catalyst or inorganic material, including a literature survey and planning.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Podrobno poznavanje izbranih vrst anorganskih materialov ter katalizatorjev in lasnosti, ki so povezane s strukturo, morfologijo in obliko posameznega materiala. Poznavanje različnih preparativnih tehnik za njihovo pripravo in raznovrstnih metod karakterizacije. Povezava teoretičnega in praktilnega znanja z izvedbo dveh različnih projektnih nalog: sinteza in karakterizacija novega materiala ter sinteza in karakterizacija katalizatorja.	Knowledge and Comprehension In-depth knowledge of selected types of inorganic materials and catalysts and their properties, which originate from the structure, morphology and shape of the material. Knowledge of different preparation techniques and characterization methods. Connection between theoretical and practical knowledge through performing two different projects: synthesis and characterisation of a new material and synthesis and characterisation of a catalyst.
Uporaba Pridobljeno znanje zna povezati in s pomočjo dosegljive literature načrtovati modificirane sintezne postopke priprave novega materiala oz. katalizatorja. Poznavanje metod karakterizacije, njihovo komplementarnost in dopolnjevanje vodijo v razumevanje vsebine znanstvenih člankov s področja materialov.	Application Integration of acquired knowledge and planning modificating synthesis routes for the preparation of a new material or catalyst with the aid of available literature. The knowledge of characterisation methods and the ways they complement one another leads to the understanding of the contents of research articles in the field of materials chemistry.
Refleksija Študent razume in utrdi razumevanje povezave med lastnostmi in sestavo ter zgradbo snovi na teoretičnem nivoju, na dveh konkretnih, samostojno izvedenih primerih pa je sposoben novo znanje uporabiti v praksi, kar vodi v samostojno načrtovanje in karakterizacijo novih materialov oz. katalizatorjev.	Analysis The student solidifies the understanding of the connections between properties, composition and structure of material on a theoretical level. Acquired knowledge is then transferred to the practical level and applied to two specific cases. This enables independent planning and characterisation of new materials and catalysts.
Prenosljive spretnosti Študent zna uporabljati zbirke podatkov, izbrati najbolj primerne sintezne postopke za	Skill-transference Ability The student is able to use databases, chooses the most appropriate synthesis routes for the

pripravo novega materiala oz. katalizatorja in ve, katere metode karakterizacije bo potreboval. Ker vseh metod karakterizacije ni mogoče individualni izvesti, se sooči s »timskim« delom. Rezultate karakterizacije zna kritično ovrednotiti in z njihovo pomočjo optimirati sintezni postopek, da bo dobljeni material izboljšal. Pisno in ustno zna poročati o rezultatih projektne naloge in jih komentirati.	preparation of a new material or catalyst and knows which characterisation methods are required. Since not all characterisation methods can be performed individually, group work is required. The student is able to critically evaluate the results obtained from characterisation and uses them as a basis for the optimisation of the synthesis procedures in order to obtain materials with the best properties. The student can report and comment on the results of the project in both written and oral form.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- predavanja - seminar - izpeljava projektne naloge	- Lectures - Seminars - Execution of one project

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pogoj za pristop k izpitu je oddano poročilo o projektu (zaključene vaje). Pisni izpit. Ocene 6-10: pozitivno, ocene 1-5: negativno.		Submitted project report (completed practice) is mandatory before the exam. Written exam. Marks 6-10: pass, marks 1-5: fail.

Reference nosilca / Lecturer's references:

Romana Cerc Korošec:

1. P. Galer, R. Cerc Korošec, M. Vidmar, B. Šket. Crystal structures and emission properties of the BF2 complex 1-phenyl-3-(3,5-dimethoxyphenyl)-propane-1,3-dione : multiple chromisms, aggregation- or crystallization-induced emission, and the self-assembly effect. Journal of the American Chemical Society, 136 (20), 7383-7394, 2014.
2. M. Sluban, N, Rozman, M. Pregelj, C. Bittencourt, R. Cerc Korošec, A. Sever Škapin, A. Mrzel, S. D. Škapin, P. Umek. Transformation of hydrogen titanate nanoribbons to TiO2 nanoribbons and the influence of the transformation strategies on the photocatalytic performance. Beilstein journal of nanotechnology, 6, 831-844, 2015.
3. R. Cerc Korošec, P. Bukovec. Optimisation of the thermal-treatment of chemically prepared electrochromic nickel oxide thin films, their electrochromic properties and structural investigations. V: P.R. SOMANI(ur.). Chromic materials, phenomena and their technological applications, (Multifunctional materials and devices). Pune: Applied Science Innovations Private Limited, str. 241-282, 2010.

Anton Meden:

1. M. VIdmar, A. Golobič, A. Meden, D. Suvorov, S. D. Škapin. Sub-solidus phase relations and a structure determination of new phases in the $CaO\text{-}La_2O_3\text{-}TiO_2$ system. *Journal of the European ceramic society*, 35, 2801-2814, 2015.
2. Y. Sadikin, K. Stare, P. Schouwink, M. B. Ley, T. Jensen, A. Meden, R. Černy. Alkali metal - yttrium borohydrides : the link between coordination of small and large rare-earth. *Journal of*

solid state chemistry, 225, 231-239, 2015.
3. F. Zupanič, B. Markoli, I. Naglič, T. Weingaertner, A. Meden, T. Bončina. Phases in the Al-corner of the Al-Mn-Be system. *Microscopy and microanalysis*, 19(5), 1308-1316, 2013.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	SPEKTROKEMIJSKA ANALIZA
Course Title:	SPECTROCHEMICAL ANALYSIS

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: K2I12

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

Nosilec predmeta / Lecturer: izr. prof. dr. Mitja Kolar / Dr. Mitja Kolar, Associate Professor

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

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:

Teoretske osnove optične spektroskopije
Vrste prehodov (Zasedenost stanj in verjetnost prehodov), Vplivi na širino spektralnih črt in njihovo intenziteto.
Spektrokemijske meritve; obravnava razmerja signal/šum, pristopi optimiranja.
Uvajanje vzorcev v atomski spektroskopiji (tekočine, trdne snovi, plini) konvencionalni in sodobni pristopi (razpršilniki, elektrotermično odparevanje, laserska ablacija), hidridne tehnike.
Pretočni sistemi v atomski spektroskopiji
Teoretski in praktični vidiki; Separacijski in koncentracijski pristopi v pretočni spektroskopski analizi.
Novejši vidiki atomske aborpcijske

Content (Syllabus outline):

Theoretical basis of optical spectroscopy
Electronic states of atoms, spectral line profiles, spectral lines intensities.
Spectrochemical measurements; signal-to noise considerations in spectroscopy, optimization approaches.
Sample introduction to atomic spectrometry (liquids, solids and gases); conventional and modern approaches (aerosol formation, electrothermal vaporization and laser ablation), hydride techniques.
Flow injection analysis in atomic spectroscopy; theoretical aspects and its role in separation and preconcentration

spekrometrije- večelementna atomska absorpcijska spektrometrija. **Značilnosti visokotemperaturnih izvorov v spektrometriji** – induktivno sklopljena plazma (ICP), mikrovalovna plazma (MP), iskra, »glow discharge« (elektronska gostota, vertikalni profili, mehanizmi vzbujanja in ionizacije...). **Optična emisijska in elementna masna spektrometrija z induktivno sklopljeno plazmo;** spektralne in nespektralne motnje, njihova kontrola in zmanjševanje, optimizacija instrumentalnih pogojev, pomen interne standarizacije. **Rentgenska spektrometrija s totalnim odbojem;** značilnosti, instrumentacija, praktična uporaba. **Spektroskopske tehnike za karakterizacijo površin** **Analizne aplikacije spektroskopskih tehnik;** semikvantitativna analiza, kvantitativna analiza, analiza trdnih vzorcev, speciacijska analitika s poudarkom na uporabi ICP-MS in povezavi s kromatografskimi tehnikami, izotopska analiza, analiza površin.	procedures. **New concepts of atomic absorption spectrometry**; high resolution continuum source AAS. **Characteristics of high temperature sources in spectrometry** - inductively coupled plasma (ICO), microwave plasma (MP), spark source, glow discharge (temperature, electronic density, vertical profile, mechanisms of excitation...). **ICP atomic emission and elemental mass spectrometry;** spectral and nonspectral interferences, selection of analytical spectral lines, optimization of instrumental parameters, importance of internal standardisation. **Total reflection X-ray spectrometry;** characteristics, instrumentation, practical application. **Spectroscopic techniques for characterization of surfaces.** Analytical applications of spectroscopic techniques: semiquantitative and quantitative analysis, analysis of solid samples, speciation analysis with focus on the use of inductively coupled plasma mass spectrometry coupled with chromatographic techniques, isotope analysis, surface analysis.

Temeljna literatura in viri / Readings:

- J. Ingle, S.R. Crouch, Spectrochemical Analysis, Prentice Hall Inc., 1992
- A. Montaser, D.W. Golighty: Induced Coupled Plasma in Analytical Spectrometry, VCH Publishers
- J. Sneddon: Sample introduction in Atomic Spectroscopy, Elsevier 1990.
- E. P. Bertin: Introduction to X-ray Spectrometric Analysis, Plenum Press, N.Y.
- J. L. Burguerra: Flow Injection Atomic Spectroscopy, Marcel Dekker

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Študenti spoznajo teoretske osnove sodobnih spektroskopskih metod. *Kompetence:* Pridobijo nekatere praktične izkušnje za delo z zahtevno instrumentacijo.	Students will acquire theoretical knowledge of modern spectroscopic methods. Competences: They will get some practical skills using of demanding instrumentation.
Predvideni študijski rezultati:	**Intended Learning Outcomes:**

Znanje in razumevanje V teoretskem delu pridobijo študenti potrebna teoretska znanja, ki so osnova za reševanje različnih praktičnih problemov.	Knowledge and Comprehension Students will gain theoretical knowledge which is the basis for solution analytical problems using spectroscopic methods.
Uporaba Pridobljeno znanje je osnova za uspešno opravljanje razvojno raziskovalnega dela na področju zahtevne analitike v različnih okoljih (okoljski laboratoriji, zahtevnejše tehnologije, biomedicinske aplikacije).	Application The obtained knowledge is basis to perform spectroscopic measurements in different research areas (environmental laboratories, modern technologies, biomedical applications).
Refleksija Študentje pridobijo znanja za kritično vrednotenje in interpretacijo spektroskopskih podatkov ter vlogo teh metod pri karakterizaciji sodobnih materialov, vzorcev iz okolja in bioloških vzorcev.	Analysis Students will gain knowledge and experiences for critical evaluation and interpretation of spectroscopic data and the role of these methods for characterization of new materials and for analysis of environmental and biological samples.
Prenosljive spretnosti Študentje se naučijo iskati in uporabljati primarno literaturo. Naučijo se kritične analize literature, sinteze podatkov, pisanja kritičnih preglednih pisnih izdelkov, ustnega poročanja.	Skill-transference Ability Students will be able to find select and use relevant literature, they will be trained to write scientific reviews and to present scientific reports.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarji, laboratorijske vaje.	Lectures, seminars and laboratory work.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni seminar s predstavitvijo,	40%	Written seminar project with oral presentation in front of the students,
Pisno poročilo o eksperimentalnem delu,	10%	Report on practical work,
Ustni izpit	50%	Oral examination

Reference nosilca / Lecturer's references:

1. HUŠ, Sebastjan, KOLAR, Mitja, KRAJNC, Peter. Separation of heavy metals from water by functionalized glycidylmethacrylate poly (high internal phase emulsions). Journal of chromatography. A, ISSN 0021-9673, 2016, vol. 1437, str. 168-175.
2. JERENEC, Simona, ŠIMIĆ, Mario, SAVNIK, Aleš, PODGORNIK, Aleš, KOLAR, Mitja, TURNŠEK, Marko, KRAJNC, Peter. Glycidyl methacrylate and ethylhexyl acrylate based polyhipe monoliths : morphological, mechanical and chromatographic properties. Reactive & functional polymers, ISSN 1381-5148. [Print ed.], 2014, vol. 78, str. 32-37.
3. KOLAR, Mitja, DOBČNIK, Danilo, RADIĆ, Njegomir. Chemically treated silver electrodes for the determination of cysteine. Mikrochimica acta, ISSN 1436-5073. [Online ed.], 2002, vol. 138, no 1-2, str. 23-27 15.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	TERMIČNA ANALIZA
Course Title:	THERMAL ANALYSIS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	**/**	**2.**	**4.**
USP Chemistry, 2nd Cycle	**/**	**2nd**	**4th**

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I05

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
15	**15**	**45 LV**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: doc. dr. Romana Cerc Korošec / Dr. Romana Cerc Korošec, 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:

1. Definicija pojma termična analiza. Termogravimetrija (TG), diferenčna termična analiza (DTA) in diferenčna dinamična kalorimetrija (DSC) – princip merjenja. Komplementarnost TG in DSC metode (termični razpad/fazni prehod).
2. Teoretske osnove termičnega razpada trdnih snovi; bazna linija pri TG in DSC krivulji.
3. Temperaturna kalibracija termoanalizatorja, kalibracija DSC instrumenta; fleksibilna kalibracija.
4. Analiza eksperimentalnih podatkov izmerjenih TG in DSC krivulj vzorcev z znano sestavo, primerjava z

Content (Syllabus outline):

1.) Definition of the concept “thermal analysis”. Thermogravimetry (TG); differential thermal analysis (DTA) and dynamic scanning calorimetry (DSC). TG and DSC as complementary methods (thermal decomposition/phase transition).
2.) Thermal decomposition of solids (theoretical principles), baseline of TG and DSC curve.
3.) Temperature calibration thermoanalyser, calibration of a DSC instrument, flexible calibration.
4.) Analysis of experimental data from TG and DSC curves, obtained from the

objavljenimi TG krivuljami; kvalitativna in kvantitativna analiza preprostih in kompleksnejših zmesi.

5. Termična analiza polimernih materialov - steklast prehod, hladna kristalizacija, spremljanje polikondenzacije duroplastnih materialov z visokotlačno DSC, termična stabilnost polimerov.
6. Termična analiza tankih plasti – posebnosti in priprava vzorca za merjenje.
7. Termična analiza kot orodje za študij materialov in optimiranje njihove toplotne obdelave; analiza farmacevtskih substanc, eksplozivnih snovi, kompozitnih materialov; primeri optimiranja toplotne obdelave materialov.

Študentje se najprej seznanijo s teoretskimi osnovami termične analize in nato vsebino preverijo na eksperimentalnih vajah v obliki projektnega dela, ki se nanaša na vsebino študentove usmeritve.

compounds with a known composition; comparison with the published curves. Qualitative and quantitative analysis of simple and more complex mixtures.

5.) Thermal analysis of polymeric materials (glass transition, cold crystallisation, following the condensation reaction of thermosets using high pressure DSC, thermal stability of polymers).
6.) Thermal analysis of thin films – peculiarities and sample preparation.
7.) Thermal analysis as a tool for studying materials and optimisation of their thermal treatment. Analysis of different types of materials including pharmaceutical substances, explosives and composites. Optimization of thermal treatment of materials (examples).

At the beginning of the course, the students are introduced to the theoretical principles of thermal analysis. These are then explored during experimental practice in the form of project work, which is related to the student's specialisation.

Temeljna literatura in viri / Readings:

- Handbook of Thermal Analysis and Calorimetry, Vol. 1 (Principles and Practice), M. E: Brown (urednik), Elsevier, Amsterdam 1998.
- Thermal methods; analytical chemistry by open learning, J. W. Dodd, K. H. Tonge, Chichester 1987.
- T. Leskelä: Thermoanalytical techniques in the study of inorganic materials, Dissertation, Helsinki 1996.

Cilji in kompetence:

Cilji: Spozna teoretske osnove termične analize in njeno uporabo na raznovrstnih področjih znanosti in tehnologije.
Kompetence: Obvlada principe v termične analize in jih zna uporabljati v praksi.

Objectives and Competences:

Objectives:Understanding of the basic theoretical principles of thermal analysis and the ability to use this method in different fields of science and technology.
Competences: Mastering the principles of thermal analysis and the ability to use them in practice.

Predvideni študijski rezultati:

Znanje in razumevanje
Študent osvoji in zna uporabljati osnovne principe termične analize (izvesti meritev,

Intended Learning Outcomes:

Knowledge and Comprehension
Applying the acquired knowledge, the student can use basic principles of thermal analysis

prebrati in komentirati rezultat). S pomočjo literature se nauči termično analizo uporabiti za reševanje kompleksnih problemov.	(performig measurement, interpret and comment a result). Thermal analysis can be used for solving more complex issues with the aid of references.
Uporaba Pridobljeno znanje zna povezati in uporabiti pri reševanju določenih problemov pri anorganskih in polimernih materialih ter farmacevtskih substancah, pri načrtovanju in optimiranju procesov v proizvodnji, ki so povezani s termično obdelavo in kontrolo kakovosti v industriji. Dobljene rezultate je sposoben kritično ovrednotiti.	Application Ability to merge the acquired knowledge and skills in order to solve certain issues in the field of inorganic and polymeric materials, pharmaceutical substances, for planning and optimising industrial processes connected with thermal treatment or quality control. Ability to critically evaluate the results obtained.
Refleksija Študent je sposoben uporabiti metode termične analize v praksi. Na osnovi pridobljenega znanja je sposoben kritično ovrednotiti izmerjene rezultate in jih primerjati z literaturnimi podatki.	Analysis Use the methods of thermal analysis in practice. On the basis of the knowledge acquired, the student is able to evaluate measured results and compare them with literature data.
Prenosljive spretnosti Študent zna uporabljati literaturne podatke, načrtovati izvedbo meritev za reševanje določenega problema in povezovati teorijo s prakso. Kadar je potrebno, zna za reševanje problema v kombinaciji s termično analizo uporabiti dodatne metode npr. spektroskopske in rentgensko difrakcijo. Na ta način spozna povezanost različnih področij. Ustno in pisno zna poročati o rezultatih meritev, jih kritično analizirati, primerjati z literaturnimi podatki ter komentirati morebitna odstopanja.	Skill-transference Ability Ability to use literature data, plan the execution of measurements to solve specific problems, and link theory with practice. Combining thermal methods with additional ones, i.e. spectroscopic and x-ray diffraction, when required. Thus, the student becomes acquainted with the interconnectedness of different fields. The student can report on the results of measurements in oral and written form, critically analyse them, compare them with literature data and comment on possible deviations.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanje - problemsko delo na seminarjih - laboratorijske vaje: meritve Priprava, izvedba in predstavitev projekta	- Lectures - Coursework during seminars - Laboratory practice: measurements - Project preparation and presentation

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

-pisni izpit -pisno poročilo izvedenih meritev -priprava in predstavitev skupinskega seminatskega dela	**60 %** **30%** **10 %**	-written examination -report on performed measurments -preparation and presentation of a project work

Reference nosilca / Lecturer's references:

- R. Cerc Korošec, P. Bukovec, B. Pihlar, J. Padežnik Gomilšek: The role of thermal analysis in optimization of the electrochromic effect of nickel oxide thin films, prepared by the sol-gel method. Part 1. - *Thermochim. acta*. **2003**, *402*, 57-67.
- R. Cerc Korošec, P. Bukovec: The role of thermal analysis in optimization of the electrochromic effect of nickel oxide thin films, prepared by the sol-gel method. Part 2. - *Thermochim. acta* **2004**, *410*, 65-71.
- R. Cerc Korošec, P. Kajič, P. Bukovec: Determination of water, ammonium nitrate and sodium nitrate content in »water-in-oil« emulsions using thermogravimetry and dynamic scanning calorimetry. - *J. therm. anal. calorim.* **2007**, *89*, 619 – 624.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	UPORABA NUMERIČNIH METOD V KEMIJI
Course Title:	NUMERICAL METHODS IN CHEMISTRY

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

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE212

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. Jurij Reščič / Dr. Jurij Reščič, Full 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):**
Ponovitev in obravnava matematičnih orodij na splošno s poudarkom na konkretnih numeričnih primerih s področja kemije. Uporaba nekaterih splošno uporabljanih programov (npr. Microsoft Excel) pri reševanju v nadaljevanju opisanih numeričnih problemov. Osnove programiranja v enem izmed višjenivojskih programskih jezikov, v katerih je napisana večina programske opreme, ki se uporablja v kemiji (Python, Fortran, C). Razčlenitev problema, prikaz poteka reševanja z blokovno shemo, opis in razlaga izbranega	Introduction into mathematical tools with applications to computational problems found mostly in chemistry. Demonstration of usage of common software (e.g. Microsoft Excel) for scientific data processing and interpretation. Basics of high -level programming language used in science (Python, Fortran and/or C).Decomposition of a given problem, block diagram flowchart, description of a chosen algorithm used to solve the problem, and designing appropriate computer code. Main topics: rounding errors, statistical analysis (mean value, standard deviation), linear

algoritma za dani problem ter konstruiranje računalniškega programa. Zaokrožitvene napake, statistični račun, regresijska analiza (korelacijski koeficienti), računanje s pomočjo rekurzijskih formul, reševanje sistemov linearnih enačb. Matrike, inverzija matrik, lastni vektorji in lastne vrednosti matrik, LU razcep, numerično reševanje nelinearnih enačb in sistema nelinearnih enačb, numerično integriranje (trapezna in Simpsonova formula, metoda Monte Carlo), numerično odvajanje, interpolacija, naključna števila, iskanje ekstremov funkcij ene in več spremenljivk (metoda zlatega reza, gradientna in simplex metoda). Numerično reševanje diferencialnih enačb 1. in 2. reda (metoda Runge-Kutta, metoda prediktor-korektor), numerično reševanje sistema diferencialnih enačb. Začetni in robni problemi. Parcialne diferencialne enačbe (difuzijska, valovna, Poissonova). Diskretna Fourierova transformacija in njena uporaba pri analizi signalov merilnih inštrumentov.	regression analysis and correlation coefficients, recursion formulae, interpolation, systems of linear equations, matrices, inversion of matrices, eigenvectors and eigenvalues, LU decomposition, solving nonlinear equations, numerical integration (Trapezoidal and Simpson's rule, Monte Carlo method), numerical differentiation, interpolation, random numbers, minimization of functions of a single and multiple variables (golden ratio search, gradient and Simplex method). Numerical solving of differential equations of 1st and 2 nd order (Euler's method, Runge-Kutta method, predictor-corrector method), systems of differential equations. Initial and boundary value problems. Partial differential equations (diffusion, wave, and Poisson's equation). Discrete Fourier transform and its usage in signal analysis, autocorrelation.

Temeljna literatura in viri / Readings:

-B. Plestenjak, Razširjen uvod v numerične metode, DMFA, Ljubljana, 2015, (15%).
- John H. Mathews, Kurtis D. Fink, Numerical methods using MATLAB 4th ed., Prentice Hall, 2004. (10%)
- W. H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery, Numerical Recipes in C/Fortran, Cambridge University Press, Cambridge, 1994. (10%)
- E. Joseph Billo, Excel for Chemists 2nded., Wiley, New York 2001. (10%)
- J. Reščič in T. Urbič, Numerične metode-praktikum, FKKT, Ljubljana, 2015.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Pri predmetu naj bi študent dobil teoretično podlago in praktične izkušnje za samostojno reševanje matematično-fizikalnih problemov z različnih področij znanosti in tehnike s posebnim poudarkom na kemiji, in to z uporabo računalnika. *Kompetence:* Praktično naj bi se naučil osnov	*Objectives:* Understanding of basic methods and algorithms used in solving computational problems encountered in various fields of chemistry. *Competences:* To learn basics of one of higher-level programming languages used for data

programiranja v enem izmed višjenivojskih programskih jezikov ter spoznal osnovne algoritme, ki se uporabljajo pri numeričnem reševanju raznih problemov. Seznanil pa naj bi se tudi s stanjem in problematiko numeričnega računanja na področjih, ki mejijo na kemijo.	analysis and high-performance computing. Usage of common software to present and interpret experimental data.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Predmet je namenjen seznanjanju z osnovnimi metodami za reševanje numeričnih problemov v naravoslovju in tehniki s posebnim poudarkom na kemiji. Študent se nauči identificirati problem, ga razčleniti in potem rešiti s pomočjo računalniškega programa, ki ga skonstruira sam.	Knowledge and Comprehension The subject is aimed toward basic numerical methods commonly used throughout various natural sciences and especialy in chemistry. A student learns to identify the problem, dissect it, and solve it using a self-developer computer program or algorithm.
Uporaba Uporabnost pridobljenega znanja je zelo široka in nikakor ni omejena samo na kemijo. Študent se je sposoben spoprijeti skoraj z vsakim numeričnim problemom, na katerega naleti med študijem ali pozneje, neodvisno od področja znanosti.	Application The acquired knowledge is widely applicable and is not only chemistry-related. A sudent is able to solve problems encountered during the study and later, independent on the field of science.
Refleksija Študent pridobi občutek, da se je sposoben lotiti poljubnega numeričnega problema, za katerega še ni (ali pa ne pozna) napisanega računalniškega programa.	Analysis A student becomes confident about her/his ability to solve a given numerical problem using a cpomputer program developer on her/his own.
Prenosljive spretnosti Spretnosti in znanje, ki si ga študent pridobi pri predmetu, so v največji meri splošne in prenosljive, uporabne na vseh področjih znanosti in tehnike, kjer so podatki in rezultati podani v numerični obliki.	Skill-transference Ability Acquired knowledge and skills are general and can therefore be used in other scientific or technical fields where numerical data are commonly used and processed.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja. - Praktične vaje na računalniku.	Lectures and computer lab course.

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

Pisni izpit. Ocene: 6-10 (pozitivno), 1-5 (negativno) ob upoštevanju Statuta UL in fakultetnih pravil.		Written exam.

Reference nosilca / Lecturer's references:

- Nosilec predmeta je eden izmed soavtorjev računalniškega programa za simulacije Molsim v programskem jeziku Fortran (avtor programa je prof. Per Linse, Univerza v Lundu, Švedska) (to je za ta predmet morda najpomembnejša referenca)
- REŠČIČ, Jurij, VLACHY, Vojko, HAYMET, A. D. J. Highly asymmetric electrolytes: beyond the hypernetted chain integral equation. *J. Am. Chem. Soc.*, 1990, vol. 112, no. 9, str. 3398-3401.
- REŠČIČ, Jurij, LINSE, Per. Gas-liquid phase separation in charged colloidal systems. *J. Chem. Phys.*, 2001, vol. 114, no. 22, str. 10131-10136.
- REŠČIČ, Jurij, LINSE, Per. Potential of mean force between charged colloids : effect of dielectric discontinuities. *The Journal of chemical physics*, 2008, vol. 129, no. 11, art. no. 114505.

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	VODE KOT HIDROGEOLOŠKI, EKOLOŠKI IN ANALIZNI SISTEM
Course Title:	WATER AS HYDROGEOLOGICAL, ECOLOGICAL, AND ANALYTICAL SYSTEM

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

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I14

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: izr. prof. dr. Nataša Gros / Dr. Nataša Gros, Associate 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:

KAKOVOST VOD
-karakterizacija vodnih virov
-definicije povezane s kakovostjo vod
-antropogeni vplivi na kakovost vod
-polucija - izvori in poti
- prostorske in časovne spremembe
-ekonomski razvoj in kakovost vod
STRATEGIJE OCENJEVANJA KAKOVOSTI VOD
-proces ocenjevanja kakovosti vod
-značilni primeri programov spremljanja kakovosti vod
-načrtovanje programov ocenjevanja
-implementacija programov ocenjevanja kakovosti vod
-vrednotenje rezultatov
-nadzor nad kakovostjo podatkov

Content (Syllabus outline):

WATER QUALITY
- characterisation of water bodies
- definitions related to water quality
- anthropogenic impacts on water quality
- pollutant sources and pathways
- spatial and temporal variations
- economic development and water quality

STRATEGIES FOR WATER QUALITY ASSESSMENT
- water quality assessment process
- typical water quality monitoring programmes
- design of assessment programmes
- implementation of water quality assessment programmes
- data processing

-interpretacija rezultatov IZBIRA SPREMENLJIVK KAKOVOSTI VOD -hidrološke spremenljivke -splošne spremenljivke -hranilne snovi -organska snov -prevladujoči ioni -druge anorganske spremenljivke -kovine -organski kontaminanti -mikrobiološki indikatorji -izbira spremenljivk PODTALNICA - značilnosti vodonosnikov - interakcije voda-prst-kamnina - vidiki kakovosti podtalnice - strategije ocenjevanja kakovosti - primeri ocenjevanj kakovosti podtalnice REKE -hidrološke značilnosti -kemijske značilnosti -biološke značilnosti -najpomembnejši vidiki kakovosti rek -strategije ocenjevanja kakovosti rečnih sistemov -pristopi k spremljanju in ocenjevanju kakovosti rečnih sistemov – študij primerov JEZERA -značilnosti in tipologija -vidiki kakovosti -strategije ocenjevanja kakovosti jezer -pristopi k ocenjevanju jezer – študij primerov ANALIZA IN INTERPRETACIJA PODATKOV O KAKOVOSTI VOD -Preverjanje zanesljivosti podatkov (anionsko-kationska bilanca, različna preverjanja, relativni odnosi med ioni) -Sklepanje na kamninski izvor -Grafične metode (»Stiff« diagram, Piper diagram) -Prepoznavanje reakcij v podtalnici	- data quality control - interpretation SELECTION OF WATER QUALITY VARIABLES - hydrological variables - general variables - nutrients - organic matter - major ions - other inorganic variables - metals - organic contaminants - microbiological indicators - selection of variables GROUNDWATER - characteristics of groundwater bodies - water-soil-rock interactions - ground water quality issues - assessment strategies - examples of ground water assessment RIVERS - hydrological characteristics - chemical characteristics - biological characteristics - major water quality issues in rivers - strategies for water quality assessment in river systems - approaches to river monitoring and assessment: case studies LAKES - characteristics and typology - water quality issues - assessment strategies - approaches to lake assessment: case studies ANALYSIS AND INTERPRETATION OF WATER QUALITY DATA - reliability of data (anion-cation balance, miscellaneous checks, relative amounts of ions reported) - source-rock deduction - graphical methods – “Stiff” diagram, Piper diagram - ground water reactions

Temeljna literatura in viri / Readings:

- Chapman, D. [Ed] 1996 *Water Quality Assesments – A Guide to Use of Biota, Sediments and Water in Environmental Monitoring – 2nd Edition*. UNESCO/WHO/UNEP, University press, Cambridge. 626 strani (Poglavja: 1-3, 6-7, 9-10 – skupaj 289 strani)

Dodatna literatura:

- Hounslow, A. W. 1995 *Water Quality Data – Analysis and Interpretation.* Lewis Publishers, Boca Raton, New York. (Poglavja: 1-4)

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Študent se pri predmetu usposobi za načrtovanje in implementacijo programov spremljanja in ocenjevanja kakovosti različnih vodnih virov. *Kompetence:* Sposobnost vrednotenja tovrstnih rezultatov, suveren nadzor nad kakovostjo pridobljenih podatkov ter za interpretacijo rezultatov.	Objectives: Knowledge and understanding necessary for planning and implementing programmes for monitoring and evaluation of water quality. Competences: Ability to evaluate and interpret water quality data.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Študent zna spremljati in ocenjevati kakovost različnih vodnih virov.	Knowledge and Comprehension Student develops knowledge and comprehension necessary for monitoring and evaluation of water quality of different water bodies.
Uporaba Uporaba pridobljenih rezultatov za suveren nadzor nad kakovostjo vodnih virov.	Application Student develops ability of using analytical data for water quality evaluation.
Refleksija Študent ima kritičen odnos do kakovosti vodnih virov.	Analysis Student adopts critical attitude towards quality of different water bodies.
Prenosljive spretnosti - sintetično analitično, ustvarjalno mišljenje in reševanje problemov - fleksibilna uporaba znanja v praksi - iniciativnost/ ambicioznost, - osebna odgovornost in odgovornost do skupine, - vrednota stalnega osebnega strokovnega napredovanja	Skill-transference Ability Student fosters: - abilities of data analysis and synthesis, innovative thinking and problem solving - abilities of using knowledge flexibly in practice situations - initiative/ambition - personal responsibility and responsibility towards a group of peers - skills of monitoring personal professional development.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja in seminar z aktivno udeležbo študentov (razlaga, vodeni razgovor, diskusija, študij primerov, reševanje problemov); Seminar: skupinsko in individualno delo povezano s pripravo izhodišč, postavitvijo hipoteze in določitvijo strategije odvzema vzorcev za projektno delo in pisanje z njim povezane seminarske naloge »Ocena kakovosti reke/jezera X in pritokov«, ustna predstavitev izhodišč seminarske naloge. Terenska vaja s prevzemanjem vlog, pri kateri se študenteje praktično usposobijo za odvzem vzorcev vod in dejavnosti na mestu odvzema; Individualni odvzem vzorcev vod v zvezi s seminarsko nalogo. Laboratorijske vaje: analiza vzorcev vod, ki so jih študentje odvzeli individualno in so povezani z njihovimi seminarskimi nalogami (za doseganje višje analizne učinkovitosti in razvijanje osebne odgovornosti in odgovornosti do skupine študentje celotno skupino vzorcev vod analizirajo timsko z delitvijo posamezni zadolžitev). Skupinsko in individualno vrednotenje analiznih rezultatov. Pisanje seminarske naloge, interpretacija rezultatov v povezavi spostavljeno hipotezo in predhodno poznanimi podatki.	Lectures and seminar with active participation of students: explanations, guided discussions, discussions, case studies and problem solving. Seminar: students by individual and group work study the context and define the hypotheses of their project entitled “Evaluation of water quality of a selected water body - river/lake X”. They design sampling strategies and suggest sampling points and prepare an oral presentation. Development of skills necessary for water sampling and on-spot measurements. Water sampling performed individually for the purpose of the project. Laboratory practical: analyses of water samples which students sampled in the context of their project. For higher laboratory efficiency and developing responsibility towards a group of peers students analyse all water samples by sharing tasks. They evaluate data quality and interpret analytical results in relation to their expectations and hypotheses, and write a project report.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
A) Seminarska naloga 40 % B) Izvedba projekta in predstavitev projektne zasnove 40 % C) Ustni izpit 20 % Skupna ocena mora biti 6 ali več (uspešno).		

Reference nosilca / Lecturer's references:

- GROS, Nataša, GORENC, Bogomil. Performance of ion chromatography in the determination of anions and cations in various natural waters with elevated mineralization. *J. chromatogr.*, 1997, vol. 770, str. 119-124.
- GROS, Nataša. The comparison between Slovene and Central European mineral and thermal waters *Acta chim. slov.*, 2003, letn. 50, št. 1, str. 57-66.
- GROS, Nataša, NEMARNIK, Andrej. Accurately determining hydrogen carbonate in water in the presence of or simultaneously with the anions of carboxylic acids. *Acta chim. slov*, 2007, vol. 54,

no. 1, str. 210-215.