

**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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**Vrsta predmeta / Course Type:** izbirni strokovni / Elective Professional

**Univerzitetna koda predmeta / University Course Code:** K2102

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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Osnovni principi zgradbe kristalov: Tipi vezi v kristalih (ionska, kovalentna, kovinska). Molekulska - Van der Waalova vez, vodikova vez in druge interakcije med molekulami (npr.  $\pi\cdots\pi$  in  $\pi\cdots\sigma$  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

**Content (Syllabus outline):**

Basic principles of crystal structure: Types of bonds (ionic, covalent, metal). Intermolecular interactions (Van der Waals, hydrogen bonds,  $\pi\cdots\pi$  and  $\pi\cdots\sigma$  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 symmetry).

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.

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:

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 and Competences:

*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:**

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.

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 projektne in timsko delo.

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.

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.

**Intended Learning Outcomes:**

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.

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.

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.

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:**

- predavanja
- praktične vaje v računalniški učilnici
- projektno delo
- individualne naloge

**Learning and Teaching Methods:**

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.		Written exam after successfully accomplished tutorials.
Ocene: 6-10 (pozitivno) in ocene 1-5: (negativno)		- Grade: 6-10 (positive) 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[[difformatotricopper(II)]-di-[mu]<sub>3</sub>-formato-tetra-[mu]<sub>2</sub>-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 LaTi<sub>2</sub>Al<sub>9</sub>O<sub>19</sub> and reanalysis of the crystal structure of La<sub>3</sub>Ti<sub>5</sub>Al<sub>15</sub>O<sub>37</sub>. *Acta crystallogr., B Struct. sci.*, 2011, vol. B67, no. 6, str. 455-460.

## UČNI NAČRT PREDMETA / COURSE SYLLABUS

<b>Predmet:</b>	ANORGANSKA KEMIJA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:****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.

**Seminar:** Določanje mehanizma anorganskih reakcij iz aktivacijske entropije in aktivacijske

**Content (Syllabus outline):****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

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 karakterizacije.

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

### 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.

### Cilji in kompetence:

*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.  
*Kompetence*: razumevanje in načrtovanje zatevnejših anorganskih reakcij.

### Objectives and Competences:

**Objectives**: to gain the in-deep understanding of principles of synthesis, reactivity, properties and application of inorganic compounds that are first covered by General and Inorganic Chemistry courses in 1<sup>st</sup> Cycle.  
**Competences**: understanding and planning of advanced inorganic reactions.

### Predvideni študijski rezultati:

#### Znanje in razumevanje

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.

#### Uporaba

Študent dobi poglobljeno teoretsko znanje, ki mu pomaga pri načrtovanju sintez spojin in predvidevanju njihovih lastnosti. Sposoben naj bi bil uporabljati svoje znanje interdisciplinarno in na praktičnih primerih.

#### Refleksija

Kemija je eksperimentalna veda in osnovni cilj solidnega teoretskega znanja naj bo njegova uporaba.

### Intended Learning Outcomes:

#### Knowledge and Comprehension

Understanding of advanced principles of the properties and reactivity of inorganic compounds Ability to understand and plan the syntheses of inorganic compound.

#### Application

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 problems that involve inorganic chemistry.

#### Analysis

Chemistry is experimental science and the goal of theoretical knowledge and theoretical research is its practical use.

<b>Prenosljive spretnosti</b> Predmet širi znanje in nakazuje interdisciplinarnost večine raziskovalnih in razvojnih dejavnosti.	<b>Skill-transference Ability</b> The course broadens the knowledge and shows the interdisciplinary nature of most research projects.
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**Metode poučevanja in učenja:**

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.).

**Learning and Teaching Methods:**

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:**

Pisni in ustni izpit: ocene od 6-10 (pozitivno) oz. 1-5 (negativno).

Delež (v %) /

Weight (in %) **Assessment:**

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  $\beta$ -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)  $\beta$ -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

<b>Predmet:</b>	BIOFIZIKALNA KEMIJA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:****Biološko pomembne molekule**

Proteini, nukleinske kisline, polisaharidi, lipidi, maščobe, surfaktanti. Struktura, funkcija in njihovo okolje v celici .

**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.

**Content (Syllabus outline):****Biologically important molecules**

Proteins, nucleic acids, polysaccharides, fats, lipids, surfactants. Structure, function and their environment in the cell.

**Proteins, nucleic acids and lipids in aqueous solution**

Water: Hydrogen bonds, structure of crystalline and liquid water. Solvation: The Born model of ion solvation, 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**

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.

### **Thermodynamics of biomolecular systems**

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:**

*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.

### **Objectives and Competences:**

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:**

#### Znanje in razumevanje

Predmet daje študentu teoretično (predavanja, seminar) in praktično (laboratorijske vaje) znanje iz osnov biofizikalne kemije. Pridobljeno znanje je nujno potrebno pri razumevanju osnov

### **Intended Learning Outcomes:**

#### Knowledge and Comprehension

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.

<p>termodinamike biokemijskih procesov na molekularnem nivoju.</p> <p><u>Uporaba</u> 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.</p> <p><u>Refleksija</u> 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.</p> <p><u>Prenosljive spretnosti</u> Študent se nauči nekaterih teoretičnih in eksperimentalnih pristopov, ki so osnova pri načrtovanju, spremljanju in vodenju eksperimentov v biokemiji.</p>	<p><u>Application</u> 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.</p> <p><u>Analysis</u> 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.</p> <p><u>Skill-transference Ability</u> Students will learn some of the theoretical and experimental approaches, which set the basis for planning and monitoring experiments in biochemistry and chemistry.</p>
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**Metode poučevanja in učenja:**

Predavanja, seminarji: z uporabo različnih učnih pripomočkov (kreda in tabla, Power Point, prosojnice).  
Vaje: skripta, teoretična navodila in praktične laboratorijske vaje.

**Learning and Teaching Methods:**

Lectures, seminars, laboratory exercises.

Delež (v %) /

Weight (in %) **Assessment:****Načini ocenjevanja:**

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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

**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.

**Content (Syllabus outline):**

**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

### **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 ozkokožno rentgensko sipanje, eksperimentalni sistemi, aplikacija, analiza in interpretacija rezultatov sipanja

### **Osmometrija**

določanje molskih mas, osmotskih koeficientov in virialnih koeficientov z različnimi 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.

signal analysis, CD - titration usefulness in the 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.

Uporaba

Uporaba kalorimetričnih, spektrometričnih in osmometričnih metod, metod sipanja in drugih fizikalnih metod za določitev fizikalnih lastnosti raznih bioloških in koloidnih

**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.

Application

Using calorimetric, spectroscopic, osmometric, scattering and other physical methods for determining the physical properties of various biological and colloidal systems, solutions and

sistemov, raznih raztopin ter fizikalnih značilnosti kemijskih reakcij oziroma procesov.	various physical properties of chemical reactions and processes.
<u>Refleksija</u> 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.	<u>Analysis</u> 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.
<u>Prenosljive spretnosti</u> Sistematičnost pristopa pri reševanju projektne naloge, zbiranje literature, ovrednotenje in poročanje o rezultatih projekta.	<u>Skill-transference Ability</u> Systematic approach to solving the experimental problems, collecting of literature, evaluating and reporting on the results of the project.

**Metode poučevanja in učenja:**

Predavanja, eksperimentalne praktične vaje, projektna vaja.

**Learning and Teaching Methods:**

Lectures, seminars, laboratory exercises.

**Načini ocenjevanja:**

Pisni izpit po uspešno opravljenih vajah. Ocene: pozitivno (6-10), negativno (1-5).

Delež (v %) /

Weight (in %) **Assessment:**

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)-dinitrobenzoyl 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 fullerenehexamalononic acid Th-C66(COOH)<sub>12</sub> 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, KOGELJ, 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.

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## 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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

**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:**

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

**Prerequisites:**

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 electrodicts. Electric double-layer. Role of water as a solvent. Hydrogen bond. Forces in solutions. Solvation 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. Hoffmeisterova 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 voltometrija, impedančna spektroskopija. Simulacija elektrodnih procesov. Mehanizem izločanja vodika (HER) in redukcije kisika (ORR).

#### *Elektrokemija materialov*

- Elektrodepozicija, elektrosinteza in tehnike za študij procesov. Samosestavljljive monoplasti-SAM, podnapetostno izločanje-UPD, elektrokemijska kvarčna mikrotehnica-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 inhibition, passivation and anticorrosion protection.

-Electrochemical energy sources (efficiency, energy density), overview of conventional and advanced systems (Zn/MnO<sub>2</sub>, Pb/PbO<sub>2</sub>, Ni/Cd, Ni/MH, Li/Li<sup>+</sup>, fuel cells), photovoltaic systems.

klasičnih in naprednih sistemov (Zn/MnO<sub>2</sub>, Pb/PbO<sub>2</sub>, Ni/Cd, Ni/MH, Li/Li<sup>+</sup>, 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, Electrode in Chemistry, Engineering, Biology, and Environmental Science*, Vol. 2B, 2<sup>nd</sup> 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, *Interfacial 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:

<p><b>Znanje in razumevanje</b> 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.</p>	<p><b>Knowledge and Comprehension</b> 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.</p>
<p><b>Uporaba</b> 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.</p>	<p><b>Application</b> 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.</p>
<p><b>Refleksija</b> 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.</p>	<p><b>Analysis</b> 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.</p>
<p><b>Prenosljive spretnosti</b> 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.</p>	<p><b>Skill-transference Ability</b> 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.</p>

**Metode poučevanja in učenja:**

Predavanja, seminarji

**Learning and Teaching Methods:**

Lectures, seminars

Delež (v %) /

**Načini ocenjevanja:**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 fullerenehexamalononic 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 fullerenehexamalononic 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 fullerenehexamalonate  $T_h-C_{66}(COONa)_{12}$ , 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.

<b>UČNI NAČRT PREDMETA / COURSE SYLLABUS</b>
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<b>Predmet:</b>	FIZIKALNA KEMIJA II
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

**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  
prof. dr. Vojeslav Vlachy / Dr. Vojeslav Vlachy, 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 sistemi.

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.

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, Langmuir and B.E.T. isotherms, ligand binding to macromolecules.

**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.

**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

**Cilji in kompetence:**

**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 globlje 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 and Competences:**

**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:**

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.

Uporaba

Pri tem predmetu se spoznamo z modernimi 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

**Intended Learning Outcomes:**

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.

Application

The students get to know the modern theoretical methods used for studying the properties of different substances. The methods are used in chemistry, pharmacy and biology, as well as in planning different technological processes, such as separation methods. The

osnova raziskovalnemu delu na področju kemije.	course is providing the bases for the research work in the chemistry field.
<u>Refleksija</u> 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.	<u>Analysis</u> 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 needed in different areas of chemistry.
<u>Prenosljive spretnosti</u> Spretnosti uporabe domače in tuje literature in drugih virov, identifikacija in reševanje problemov, kritična analiza rezultatov, kvantitativno razumevanje drugih (bolj opisnih) predmetov.	<u>Skill-transference Ability</u> 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:**

- Predavanja, seminarji.

**Learning and Teaching Methods:**

- Lectures  
- Seminars

Delež (v %) /

**Načini ocenjevanja:**

Weight (in %) **Assessment:**

Pisni (nadomestita ga lahko dva pozitivno ocenjena kolokvija) in ustni izpit.		Written and oral exam.
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**Reference nosilca / Lecturer's references:**

- DILL, Ken A., TRUSKETT, Thomas Michael, VLACHY, Vojko, **HRIBAR-LEE, Barbara**. Modeling water, the hydrophobic effect, and ion solvation. *Annu Rev Biophys Biomol Struct*, 2005, vol. 34, str. 173-199.

- JARDAT, Marie, **HRIBAR, Barbara**, VLACHY, Vojko. Self-diffusion of ions in charged nanoporous media. *Soft matter*, 2012, vol. 8, no. 4, str. 954-964.

- **HRIBAR, Barbara**, LUKŠIČ, Miha, VLACHY, Vojko. Partly-quenched systems containing charges. Structure and dynamics of ions in nanoporous materials. *Annu. rep. prog. chem. Sect C. Phys. chem*, 2011, vol. 107, no. 1, str. 14-46

- B. Jamnik and V. Vlachy, *Ion Partitioning between Charged Micropores and Bulk Electrolyte Solution. Mixtures of Mono- and Divalent Counterions and Monovalent Co-Ions*, *J. Am. Chem. Soc.* **117**, 8010– 8016 (1995).

- B. Hribar and V. Vlachy, *Evidence of Electrostatic Attraction between Equally Charged Macroions Induced by Divalent Counterions*, *J. Phys. Chem. B* **101**, 3457– 3459 (1997).

- V. Vlachy, *Ionic Effects Beyond the Poisson-Boltzmann Theory*, *Annu. Rev. Phys. Chem.* **50**, 145– 165 (1999).

## UČNI NAČRT PREDMETA/COURSE SYLLABUS

<b>Predmet:</b>	FOTOKEMIJA IN RADIKALI
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

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: prof. dr. Darko Dolenc / Dr. Darko Dolenc, 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:**  
**Organska fotokemija.**  
a) Uvod. Absorpcija svetlobe, elektronska stanja in prehodi, lastnosti vzbujenih stanj. Fluorescenca, fosforescenca, Jablonskijev diagram, kvantni izkoristek. Prenos energije, dušenje.  
b) Fotokemične reakcije. Adicije, substitucije, eliminacije, fragmentacije, premestitve, izomerizacije, cikloadicije, oksidacije in redukcije.  
c) Fotokemične reakcije v okolju (ozračje, vode).  
**Kemija radikalov.**

**Content (Syllabus outline):**  
**Organic photochemistry**  
a) Introduction: absorption of light, electronic states and transitions, properties of excited states. Fluorescence, phosphorescence, Jablonski diagram, quantum yield. Energy transfer, quenching.  
b) Photochemical reactions: Additions, substitutions, eliminations, fragmentations, rearrangements, cycloadditions, oxidations and reductions  
c) Environmental photochemistry (atmosphere, waters)  
**Chemistry of radicals**  
a) Introduction: Properties of radicals, reactivity and stability, delocalization and electronic effects, formation of radicals.



- a) Uvod. Lastnosti radikalov. Reaktivnost in stabilnost radikalov, delokalizacija in 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.  
d) Pomembne radikalske reakcije v organski sintezi.

#### **Polimeri**

- a) Polimerizacija (radikalska, ionske, koordinacijska, ATRP).  
b) Osnove strukture polimerov, kopolimeri, funkcionalni polimeri.  
c) Reakcije na polimerih (zamreženje, graft polimerizacija).  
d) Pretvorbe funkcionalnih skupin

- 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) Polymerization reactions (radical, ionic, coordination, ATRP).  
b) Basics of polymer structure, copolymers, functional polymers.  
c) Reactions on polymers (crosslinking, graft polymerization).  
d) Transformation of functional groups.

#### **Temeljna literatura in viri / Readings:**

- A. Gilbert, J. Baggott, *Essentials of Molecular Photochemistry*, Ellis Horwood, 1991 (30%).  
J. Fossey, D. Lefort, J. Sorba, *Free radicals in organic chemistry*, J. Wiley and Sons, 1995 (50%).  
M. P. Stevens, *Polymer Chemistry*, Oxford University Press, 1999 (20 %).

#### **Cilji in kompetence:**

##### Cilji predmeta

Študent nadgradi znanja iz področij fotokemije in kemije radikalov in polimerov. Predmet seznanja 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.

#### **Objectives and Competences:**

##### 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:**

##### Znanje in razumevanje

Poznavanje narave in uporabe fotokemičnih procesov ter pomen fotokemičnih reakcij v okolju.

#### **Intended Learning Outcomes:**

##### Knowledge and Comprehension

Characteristics of photochemical processes, their uses and importance of photochemical reactions in the environment.

Lastnosti radikalov. Značilnosti radikalskih procesov, uporaba radikalskih reakcij v sintezi. Neželjeni procesi in preprečevanje. Osnovne lastnosti in reakcije pridobivanja polimerov, modifikacije in uporaba polimerov v kemiji.	Properties of radicals. Characteristics of radical reactions, use in synthesis. Undesired radical processes and their inhibition. Basics of syntheses of polymers, modification and uses of polymers in chemistry.
<u>Uporaba</u> 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.	<u>Application</u> 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.
<u>Refleksija</u> 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.	<u>Analysis</u> Student will be able to distinguish photochemical and thermal processes, as well as radical and ionic ones.
<u>Prenosljive spretnosti</u> -Dostopanje do literaturnih virov -Zbiranje, interpretacija in kritično vrednotenje podatkov -Identifikacija in reševanje problemov	<u>Skill-transference Ability</u> Access to literature sources. Collection, interpretation and critical assessment of scientific information. Problem identification and solving.

**Metode poučevanja in učenja:**

Predavanja, seminarji, laboratorijske vaje

**Learning and Teaching Methods:**

Lectures, seminar, laboratory work

**Načini ocenjevanja:**

Delež (v %) /

Weight (in %) **Assessment:**

Pisni izpit po uspešno opravljenem praktičnem delu	100	Written exam after completed practical work
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**Reference nosilca / Lecturer's references:**

1. DOLENC, Darko, HAREJ, Maja. Direct conversion of bromohydrins to ketones by free radical elimination of hydrogen bromide. <i>J. Org. Chem.</i> , <b>2002</b> , 67, 312–313.
2. DOLENC, Darko, PLESNIČAR, Božo. Abstraction of iodine from aromatic iodides by alkyl radicals : steric and electronic effects. <i>J. Org. Chem.</i> , <b>2006</b> , 71, 8028-8036.
3. HAREJ, Maja, DOLENC, Darko. Autoxidation of hydrazones. Some new insights. <i>J. Org. Chem.</i> , <b>2007</b> , 72, 7214-7221.

4. LAVTIŽAR, Vesna, GESTEL, Cornelis A. M. van, DOLENC, Darko, TREBŠE, Polonca. Chemical and photochemical degradation of chlorantraniliprole and characterization of its transformation products. *Chemosphere*, **2014**, *95*, 408–414.

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EFKKT

**UČNI NAČRT PREDMETA / COURSE SYLLABUS**

<b>Predmet:</b>	KARAKTERIZACIJA IN STABILNOST MATERIALOV KULTURNE DEDIŠČINE
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	4 <sup>th</sup>

**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
30	30	/	/	15	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:**

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

**Prerequisites:**

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 starih 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<sub>2</sub>, ozona, NO<sub>x</sub>.  
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. Thermoxydation. Degradation processes of materials influenced by oxygen, autoxidation, antioxidants. Photolysis and photodegradation. The influence of pollutants. Influence of SO<sub>2</sub>, ozone, NO<sub>x</sub>.  
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.  
Metode za karakterizacijo materialov kulturne dediščine.  
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.  
Monitoring okoljskih parametrov  
Senzorji za svetlobo, indikatorji (dozimetri) in analize 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.  
Methods for cultural heritage material characterisation.  
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.  
Monitoring of environmental parameters.  
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:**

*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.

#### **Objectives and Competences:**

**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.
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**Predvideni študijski rezultati:**

<p><u>Znanje in razumevanje</u> 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.</p>
<p><u>Uporaba</u> Študent bo znal uporabiti principe oz. zakonitosti na primerih, ter znal poiskati povezave s prakso. Znal bo utemeljiti razvoj novih postopkov stabilizacije.</p>
<p><u>Refleksija</u> Znal bo kritično ovrednotiti skladnosti med prakso in teorijo, neskladnosti bo znal evaluirati.</p>
<p><u>Prenosljive spretnosti</u> - 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</p>

**Intended Learning Outcomes:**

<p><u>Knowledge and Comprehension</u> 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.</p>
<p><u>Application</u> To gain application of principle on real cases and to find connections with practical use. To validate development of new conservation procedures.</p>
<p><u>Analysis</u> To critically evaluate consistency between theory and practice and to evaluate differences</p>
<p><u>Skill-transference Ability</u> - 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</p>

**Metode poučevanja in učenja:**

<p>Predavanja in seminar z aktivno udeležbo študentov (razlaga, razgovor, diskusija, študij primerov, reševanje problemov); Seminar: skupinsko in individualno projektno delo na izbrano tematiko, pisanje seminarske naloge, ustna predstavitev.</p>
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**Learning and Teaching Methods:**

<p>Lectures Seminar:team and individual project work on selected theme, writing of seminar, oral presentation. Other activities: presentation of case-studies, discussion.</p>
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**Načini ocenjevanja:**

	Delež (v %) / Weight (in %)	Assessment:
Seminar	40%	Seminar
Pisni izpit	60%	Written exam

Ocenjevanje: 6-10 (pozitivno), 1-5 (negativno)		Grading scale: 6-10 (positive), 1-5 (negative)
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**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 plateau of Qumran. *Archaeometry*, 53 (2011) 791-808.

<b>UČNI NAČRT PREDMETA / COURSE SYLLABUS</b>
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<b>Predmet:</b>	KEMOMETRIJA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

<b>Vrsta predmeta / Course Type:</b>	izbirni strokovni / Elective Professional
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<b>Univerzitetna koda predmeta / University Course Code:</b>	K2I11
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Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	15	15 SV	/	/	75	5

<b>Nosilec predmeta / Lecturer:</b>	izr. prof. dr. Matevž Pompe / Dr. Matevž Pompe, Associate Professor
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<b>Jeziki / Languages:</b>	<b>Predavanja / Lectures:</b> slovenski / Slovenian
	<b>Vaje / Tutorial:</b> 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:**

**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

**Content (Syllabus outline):**

**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



Obravnavali bomo kalibracijsko premico na primeru enakih ali neenakih varianc v merskem prostoru. Poudarek bo na kasnejšem testiranju modela ter izračunu merske negotovosti ob upoštevanju enačbe premice.

#### **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.

#### **Transformacije merskega prostora**

Predstavili bomo nekatere pogoste transformacije merskega prostora (npr. PCA,...), ki jih uporabljamo za boljše predstavitev več dimenzionalnih merskih prostorov.

#### **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.

#### **Grupiranje**

Predstavili bomo enostavne postopke grupiranja podatkov v večdimenzionalnem merskem prostoru, kot tudi uporabo umetnih nevronskih mrež v te namene.

#### **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.

#### **Matematične reprezentacije kemijskih struktur**

Spoznali bomo nekatere enostavne reprezentacije kemijskih struktur, ki jih lahko

variances in metric space. The focus will be on model validation and measurement uncertainty calculation taking into account the calibration line equation.

#### **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.

#### **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.

#### **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.

#### **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.

#### **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.

#### **Mathematical representation of chemical structures**

Some simple representations of chemical structures that can be used in modeling the

uporabljam pri modeliranju povezav med 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:

*Cilji:* a) Seznaniti študente s teorijo in uporabo kemometričnih 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 and Competences:

##### 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:

##### Znanje in razumevanje

Študent se bo naučil kritično uporabljati kemometrične metode. Razumeti bo moral njihovo delovanje. Pri predmetu bo spoznal njihove bistvene prednosti ter omejitve.

##### Uporaba

Znanja bodo uporabljena v analiznih laboratorijih za zagotavljanje kakovosti

#### Intended Learning Outcomes:

##### Knowledge and Comprehension

The students will learn to critically apply chemometric methods. They will understand their operation as well as their main advantages and limitations.

##### Application

Knowledge will be used in analytical laboratories to ensure the quality of the results.

rezultatov. Prav tako se bodo znanja uporabljala pri raziskavah v okolju ter analizi živil za razpoznavanje vzorcev ter izdelavi napovednih modelov.	The obtained knowledge will be used in the environmental and food research for pattern recognition and the creation of predictive models.
<u>Refleksija</u> Študent bo sposoben samostojno obdelovati eksperimentalne podatke v večdimenzionalnem vektorskem prostoru, v njih poiskati skrite vzorce ter izdelati in validirati enostavne linearne modele.	<u>Analysis</u> 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.
<u>Prenosljive spretnosti</u> Študenti se naučijo kritično podajati in interpretirati eksperimentalne rezultate in izdelati ter validirati enostavne modele.	<u>Skill-transference Ability</u> Students learn to critically present and interpret experimental results and to create and validate simple models.

**Metode poučevanja in učenja:**

Predavanja s seminarji.

**Learning and Teaching Methods:**

Lectures and seminar work.

**Načini ocenjevanja:**Pisni in ustni izpit.  
ocene od 6-10 (pozitivno) oz. 1-5  
(negativno).

Delež (v %) /

Weight (in %)

**Assessment:**

Written and oral exam

Grades: positive 6-10; negative 1-5.

**Reference nosilca / Lecturer's references:**

- POMPE, Matevž**, DAVIS, Joe M., SAMUEL, Clint D. Prediction of thermodynamic parameters in gas chromatography from molecular structure : hydrocarbons. *J. chem. inf. comput. sci.*, 2004, vol. 44, no. 2, str. 399-409.
- 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.
- 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

<b>Predmet:</b>	KOORDINACIJSKA KEMIJA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

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 poudarkom na:  
- določanju čistosti in istovetnosti snovi z znano spojino  
- ugotavljanju vrste kemijskih vezi v spojinu  
- določanju načina koordinacije ligandov  
- opisu koordinativne sfere kovinskega iona  
- primerjavi strukturnih in analiznih podatkov s podatki kemijsko sorodnih spojin

**Content (Syllabus outline):**

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

Splošne vsebine bodo predelali na predavanjih in seminarjih, praktične na vajah v laboratoriju. Vsebina vaj: Sinteza koordinacijskih 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 predstavi 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.

- A comparison of structural and analytical data with chemically related compounds  
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:

*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.

#### Objectives and Competences:

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 shall 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.
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**Predvideni študijski rezultati:**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.

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.

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.

Prenosljive spretnosti

Po končanem študiju bo izpeljava načrtane 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.

**Metode poučevanja in učenja:**

Projektno delo v manjših skupinah.

**Intended Learning Outcomes:**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.

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.

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.

Skill-transference Ability

A derivation of the planned tasks, base on the set plan, shall 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.

**Learning and Teaching Methods:**

Seminar and laboratory project work in small groups

**Načini ocenjevanja:**

Delež (v %) /

Weight (in %) **Assessment:**

Pisni izpit po uspešno opravljenem praktičnem delu.		Written exam after practical work successfully completed.
Ocene: pozitivno 6-10		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](https://doi.org/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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup> and 4 <sup>th</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Magistrsko delo se opravlja na področju kemije. Vsebina in naslov se določata v soglasju z izbranim mentorjem – nosilcem ene izmed vsebin v programu.

**Content (Syllabus outline):**

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:**

*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.

**Objectives and Competences:**

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 finding solutions, thus proving that specific



**Kompetence:** Pri delu bo pokazal, da je pridobil večino kompetenc navedenih v programu študija.

competences from other courses have been acquired.

**Predvideni študijski rezultati:**

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.

Uporaba

Znanje in pridobljene veščine bo magistrant lahko uporabil pri opravljanju poklica.

Refleksija

Povezovanje vseh pridobljenih teoretičnih znanj z reševanjem problemov na področju kemije ter kritični pogled na uporabnost teh znanj.

Prenosljive spretnosti

Pri delu bo magistrant pridobil znanja o metodah reševanja kompleksnih problemov, o načinu prezentacije teh znanj v pisani in govornjeni obliki, povezani z ostalimi metodami posredovanja raziskav, ugotovitev itd.

**Intended Learning Outcomes:**

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.

Application

Acquired skills are necessary for professional work.

Analysis

Integration of knowledge from different topics from chemistry and supporting sciences; Development of a critical view on the knowledge applicability.

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:**

Individualno delo mentorja in samostojno študijsko in raziskovalno delo.

**Learning and Teaching Methods:**

Independent research work supervised by the mentor.

Delež (v %) /

**Načini ocenjevanja:**

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.

Weight (in %) /

**Assessment:**

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

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		positive and 1 -5 negative ( 6-pass, 7-fair, 8 and 9-very good, 10-excellent).
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**Reference nosilca / Lecturer's references:**

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UL EFKT

## 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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

**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

**Content (Syllabus outline):**

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 independent Schroedinger equation.

<p>toplotne enačbe, lastne funkcije), Fourierove vrste.</p> <p><b>Fourierova transformacija:</b> 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)</p> <p><b>Verjetnost in statistika:</b> 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</p>	<p>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.</p>
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**Temeljna literatura in viri / Readings:**

<ol style="list-style-type: none"><li>1. Josip Globevnik in Miha Brojan: Analiza II, FMF, 2012 (Poglavje dvojni in trojni integral).</li><li>2. Anton Suhadolc: Metrični prostor, Hilbertov prostor, Fourierova analiza, Laplaceova transformacija, DMFA 1998 (poglavji Fourierove vrste in Fourierova transformacija).</li><li>3. Milan Hladnik: Verjetnost in statistika, Založba FE in FRI, 2002 (poglavje Verjetnost in statistika)</li></ol> <p><b>Dopolnilna literatura:</b></p> <ol style="list-style-type: none"><li>1. P. Mizori-Oblak: Matematika za študente tehnike in naravoslovja, 2. Del FS, 1997.</li><li>2. H. P. Greenspan, D.J. Benney / J.E. Turner: Calculus: an introduction to applied mathematics, McGraw-Hill, Toronto, 1986</li><li>3. Rajko Jamnik: Matematika, DMFA Slovenije, 1994.</li><li>4. Bojan Magajna, <a href="http://www.fmf.uni-lj.si/~magajna/Matematika2KEM/osnovna.htm">http://www.fmf.uni-lj.si/~magajna/Matematika2KEM/osnovna.htm</a></li></ol>
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**Cilji in kompetence:**

<p><i>Cilj predmeta:</i> 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.</p> <p><i>Predmetno specifične kompetence:</i> Pridobljeno znanje bo študentu omogočilo globlje razumevanje nekaterih področij kemije. Na primer, dobrega razumevanja</p>
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**Objectives and Competences:**

<p>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.</p> <p>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.</p>
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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:**

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.

Uporaba  
V naravoslovju (npr. verjetnosti v kinetični teoriji plinov, Fourierove transformacije v kvantni fiziki in kemiji...)

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.

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.

**Intended Learning Outcomes:**

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.

Application  
Probability is used in the theory of gasses, Fourier transform in quantum physics and chemistry and so on.

Analysis  
The mathematics contained in the proposed course is useful in studying problems in chemistry and physics.

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:**

- Predavanja, vaje, sodelovalno učenje /poučevanje.

**Learning and Teaching Methods:**

Lectures, tutorial, homework, consultations

**Načini ocenjevanja:**

(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. opravljen/ ni opravljen; ob upoštevanju Statuta UL in fakultetnih pravil.

Delež (v %) /

Weight (in %) **Assessment:**

(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**

<b>Predmet:</b>	METODE SIPANJA ZA DOLOČANJE STRUKTURE IN DINAMIKE V NANOSISTEMIH
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

**Vrsta predmeta / Course Type:** izbirni strokovni / Elective Professional

**Univerzitetna koda predmeta / University Course Code:** K2120

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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

**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 ozkokotnega nevtronskega

**Content (Syllabus outline):**

**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.

sipanja: kontrast in variacija kontrasta, 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:**

*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

#### **Objectives and Competences:**

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



- pridobitev eksperimentalnih veščin za 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

- The acquisition of skills for the experimental measurement of small-angle scattering and 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:**

#### 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.

#### 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).

#### 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.

### **Intended Learning Outcomes:**

#### 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.

#### 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).

#### 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**

Zbiranje in uporaba znanstvenih člankov pri projektnem (raziskovalnem) delu. Poročanje o predelani literaturi, predstavitev rezultatov projektnih vaj, ter pisanje poročila v obliki znanstvenega članka.

**Skill-transference Ability**

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:**

Predavanja, seminarji, projektne laboratorijske vaje.

**Learning and Teaching Methods:**

Lectures, seminars, and laboratory practice.

**Načini ocenjevanja:**

- Pisni izpit
- Predstavitev rezultatov projektnih vaj

Ocenjevanje: 6-10 (pozitivno); 1-5 (negativno).

Delež (v %) /

Weight (in %) **Assessment:**

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

<b>Predmet:</b>	MODELIRANJE KEMIJSKIH SISTEMOV
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	4 <sup>th</sup>

**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	/	/	/	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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

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 sistemov v Hartree-Fockovem približku, primer helijevega atoma in vodikove molekule. Predstavitev in reševanje difuzijskih

**Content (Syllabus outline):**

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 Boltzmann 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 integralnih enačb. Modeliranje slučajnih procesov. Numerično integriranje s pomočjo Monte Carlo metode in Monte Carlo simulacije preprostih tekočin (Metropolisov algoritem). Molekulska dinamika preprostih kemijskih sistemov.

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:

*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 vsakodnevem delu na različnih področjih znanosti in tehnike s posebnim poudarkom na kemijo.

#### Objectives and Competences:

*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:

##### 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.

##### Uporaba

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

#### Intended Learning Outcomes:

##### Knowledge and Comprehension

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.

##### Application

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

med študijem ali pozneje, neodvisno od področja znanosti.	might find during the study and later in any kind of field of science.
<u>Refleksija</u> Študent pridobi občutek, da se je sposoben lotiti poljubnega problema in si pri tem pomagati z računalniškimi programi.	<u>Analysis</u> Student gets the feeling that he is capable of solving any kind of problem with help of computer programming.
<u>Prenosljive spretnosti</u> 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.	<u>Skill-transference Ability</u> 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:**

Predavanja, seminarji, praktične vaje na računalniku.

**Learning and Teaching Methods:**

Lectures, seminars and practical work on computers.

**Načini ocenjevanja:**

- projekt  
- seminarske in domače naloge  
Ocene: 6-10 (pozitivno), 1-5 (negativno) ob upoštevanju Statuta UL in fakultetnih pravil.

Delež (v %) /

Weight (in %) **Assessment:**

- final project  
- seminars and homeworks  
Grades: 6-10 (positive), 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

<b>Predmet:</b>	MODERNE METODE ORGANSKE SINTEZE
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

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 uporabljenih zaščitnih skupin.  
**Stereoselektivnost.** Osnovni principi stereoselektivne in asimetrične sinteze.

**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.

Stereoselektivne nekatalitske reakcije.  
Asimetrične katalitske reakcije in asimetrična organokataliza.

**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*, 3<sup>rd</sup>, 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:**

*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,

**Objectives and Competences:**

**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

-načrtovanje in sinteza kombinatornih knjižnic.

- Planning and synthesis of combinatorial libraries

**Predvideni študijski rezultati:**

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

Uporaba

Racionalno načrtovanje in praktična izvedba organskih sintez (usmerjene in ciljne sinteze organskih spojin in sinteze kombinatornih knjižnic).

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.

Prenosljive spretnosti

-Dostopanje do literaturnih virov  
-Zbiranje, interpretacija in kritično vrednotenje podatkov  
-Identifikacija in reševanje problemov  
-Poročanje (pisno in ustno)  
-Kritična analiza, sinteza

**Intended Learning Outcomes:**

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

Application

Rational planning and practical performance of organic syntheses (directed and target synthesis of organic compounds and the synthesis of combinatorial libraries)

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.

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:**

Predavanja, seminarji in vaje

**Learning and Teaching Methods:**

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)	<b>30 %</b> <b>70 %</b>	Seminar work, oral exam Grades: 6-10 (positive), 1-5 (negative)
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**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](https://doi.org/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

<b>Predmet:</b>	MODERNE NMR METODE
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

**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
45	/	30 LV	/	/	75	5

**Nosilec predmeta / Lecturer:** prof. dr. Andrej Petrič / Dr. Andrej Petrič, 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.** 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 <sup>1</sup>H in <sup>13</sup>C, programska oprema za napoved kemijskih premikov.

**Content (Syllabus outline):**

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,

**Merjenje NMR spektra.** Magnet, CW in pulzni način, zajemanje podatkov, FID, Fourierjeva 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 ( $^1\text{H}$ ,  $^{13}\text{C}$ , X); 2D eksperimenti (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).

Continuous wave and pulse mode, data acquisition, FID, Fourier transformation, 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 Overhauser 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 ( $^1\text{H}$ ,  $^{13}\text{C}$ , X), two-dimensional experiments (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).

#### **Temeljna literatura in viri / Readings:**

- J. B. Lambert, *Nuclear Magnetic Resonance Spectroscopy. An Introduction to Principles, Applications, and Experimental Methods*, Pearson Education Inc., New Jersey, 2003; 293 od 341 strani.

#### Praktikum

- S. Braun, H.-O. Kalinowski, S. Berger, *150 and More Basic NMR Experiments*, Wiley-VCH Publishers, Weinheim, 1998.

#### *Dodatna literatura*

- R. S. Macomber: *A Complete Introduction to Modern NMR Spectroscopy*, J. Wiley & Sons, Inc., New York, 1998.

- E. Derome, *Modern NMR Techniques for Chemistry Research*, Pergamon Press, Oxford, 1987.

- M. Hesse, H. Meier, B. Zeeh, *Spectroscopic Methods in Organic Chemistry*, G. Thieme Verlag, 2008

- A. Petrič: *Moderne NMR metode (interno študijsko gradivo)*, UL FKKT, 2012 (144 str.).

#### **Cilji in kompetence:**

**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

#### **Objectives and Competences:**

**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.

eksperimentov, njihovo praktično izvedbo in interpretacijo rezultatov.

**Competences:** Ability to design, perform, and interpret NMR experiments for the determination of structure and conformation of compounds in solution.

**Predvideni študijski rezultati:**

Znanje in razumevanje

Poznavanje principov in praktične izvedbe modernih NMR eksperimentov za določanje strukture in konformacije spojin v raztopini.

Uporaba

Študent uporabi pridobljeno znanje NMR spektroskopskih tehnik pri reševanju raziskovalnih problemov.

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.

Prenosljive spretnosti

Pri predmetu se študenti se izurijo v načrtovanju in izvedbi eksperimentov ter kritični interpretaciji rezultatov.

**Intended Learning Outcomes:**

Knowledge and Comprehension

Understanding the basic principles and practical knowledge about NMR experiments.

Application

Student utilizes the acquired knowledge in solving research problems

Analysis

Student applies the acquired NMR spectroscopy knowledge and skills in solving research problems.

Skill-transference Ability

Student is trained in planning and utilization of NMR spectroscopic methods, analytical thinking and using literature sources.

**Metode poučevanja in učenja:**

Predavanja in vaje

**Learning and Teaching Methods:**

Lectures and practical laboratory work

Delež (v %) /

**Načini ocenjevanja:**

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:**

- AMBROŽIČ, Gabriela, ČEH, Simon, PETRIČ, Andrej. NMR proof of a piperidine to pyrrolidine ring contraction during nucleophilic substitution. *Magn. Reson. Chem.* **1998**, *36*, 873-877.
- PETRIČ, Andrej. <sup>13</sup>C and <sup>1</sup>H NMR assignments for (1R)-3-phenyl-8-methyl-8-azabicyclo [3.2.1] octane 2-carboxylic acid methyl ester. *Magn. Reson. Chem.* **1994**, *34*, 393-394.
- PETRIČ, Andrej, BARRIO, Jorge R. Synthesis and NMR characterization of 4-[(2-tetrahydropyranyloxy)methyl]piperidine and intermediates. *J. Heterocycl. Chem.* **1994**, *31*, 545-548.

**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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

**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:**Študent oz. kandidat mora imeti predmet  
opredeljen kot študijsko obveznost.**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Ponovitev osnov kvantne mehanike ter fizike atomov in molekul (Schrödingerjev in Heisenbergov pristop, Schrödingerjeva enačba, Paulijev izključitveni princip). Opis in reševanje modelnih primerov: delec in pregrade, togi rotator, harmonski oscilator, vodikov atom. Metode za približno računanje: variacijska metoda in metoda motenj. Modeli za obravnavanje molekulskih sistemov: teorija valenčnih vezi in teorija molekulskih orbital, Hartree-Fockov model. Pregled metod, sistemov in ciljev modeliranja. Elektronska struktura: ab initio, semiempirične metode, gostotni funkcionali. Molekulska

**Content (Syllabus outline):**

Recurrence of the basics of quantum mechanics of atoms and molecules (Schrödinger's and Heisenberg's approach, Schrödinger equation, Pauli exclusion principle). Description of basic quantum mechanical models and principles, solving various relevant problems as such as particle in potential box, rigid rotor, harmonic oscillator, hydrogen atom. Methods for approximative computations: the variational principle and perturbation theory. Modelling of molecular systems: valence bond theory and molecular orbital theory, Hartree-Fock model. Review of methods, systems and objectives of molecular modeling. Molecular electronic structure: ab initio and semiempirical methods,

mehanika, molekulska dinamika, Monte Carlo. Pomen in uporaba grafike pri modeliranju. Skupine sistemov, primerne za modeliranje: manjše molekule v vakuumu, vpliv okolice, interakcije med molekulami, modeliranje kemijskih reakcij (prehodna stanja), pomoč eksperimentalnim rezultatom z metodami modeliranja.

Področje dela računalniške kvantne kemije, glavne metode in računski modeli, pregled pomembnih računalniških sistemov na tem področju, prikaz praktičnega dela z računalnikom na konkretnem problemu, individualno obravnavanje enostavnejših primerov s pomočjo metod kvantne kemije.

density functional theory. Force field based methods: Molecular mechanics, molecular dynamics, Monte Carlo method. Molecular graphics and its importance for molecular modeling. Systems for molecular modeling: small molecules in vacuo, solvent effect, intra and inter-molecular interactions, modeling of chemical reactions (transition states). Know how to use a molecular modeling as a support of laboratory experiments. Overview of methods and computer programs for molecular modeling and/or quantum chemical computations. Practical work with the computer on relevant problems from the field of molecular modeling and/or quantum chemistry.

#### Temeljna literatura in viri / Readings:

- A.R. Leach, Molecular Modelling, Principles and Applications, Addison Wesley Longman, London 1998, 585 str., (34 %)
- A. Hincliffe, Molecular Modelling for Beginners, Wiley, Chichester 2003, 401 str., (50 %)

#### Dopolnilna literatura:

- J. Koller, Struktura atomov in molekul – osnove kvantne mehanike, atomi, FKKT, Ljubljana 2002, 117 str.
- J. Koller, Struktura atomov in molekul – molekule, osnove spektroskopije, FKKT, Ljubljana 2000, 114 str.
- Priročniki za uporabo računalniških programov

#### Cilji in kompetence:

*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 molekularnem modeliranju. Pregled najbolj znanih računalniških programov za uporabo pri modeliranju (Gaussian, Spartan, HyperChem ...), prikaz praktičnega dela na osebem računalniku, delovni postaji in velikem računalniku (preko računalniške mreže). Sistematični pregled celotne snovi.

#### Objectives and Competences:

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 computer working station and big cluster (using web interface).

**Predvideni študijski rezultati:**

Znanje in razumevanje

Predmet je namenjen nadgradnji znanja kvantne kemije in njeni praktični uporabi. Študente seznanja 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.

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.

Refleksija

Študent si pridobi občutek, da se lahko v primeru nepremostljivih eksperimentalnih težav še vedno zateče k računu, kjer so problemi drugačni in navadno drugače, kar pogosto privede do zadovoljive razjasnitve problema.

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.

**Intended Learning Outcomes:**

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 tool that serves 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 computational chemistry approach.

Application

The student is able to use quantum chemistry knowledge for modeling of certain chemistry or biochemistry 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.

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.

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:**

- Predavanja
- Seminar (računske naloge iz predelane snovi)
- Praktične vaje na računalniku

**Learning and Teaching Methods:**

- Lectures
- Seminars
- Laboratory Lessons (Using computer)

Delež (v %) /

**Načini ocenjevanja:**Weight (in %) **Assessment:**

Ustni izpit	<b>60 %</b>	Oral exam
Seminarska naloga	<b>40 %</b>	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, SENECCI, 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.jmngm.2010.09.008. [COBISS.SI-ID 34621701]



**UČNI NAČRT PREDMETA / COURSE SYLLABUS**

<b>Predmet:</b>	NAPREDNE INŠTRUMENTALNE ANALIZNE TEHNIKE
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

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: izr. prof. dr. Helena Prosen / Dr. Helena Prosen, Associate Professor  
izr. prof. dr. Matevž Pompe / Dr. Matevž Pompe, Associate Professor

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

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

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

Prerequisites:

The course has to be assigned to the student.

Vsebina:

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,

Content (Syllabus outline):

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.

tandemska masna spektrometrija. Aplikacije 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 analize 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

#### Dodatna literatura:

- F. Rouessac, A. Rouessac, Chemical Analysis, Modern Instrumentation Methods and Techniques, J. Wiley & Sons, Ltd, Chichester, 2000.

- pregledni znanstveni članki iz posameznih področij / scientific review articles from different fields

#### **Cilji in kompetence:**

Študenti se seznanijo s kemometričnimi in numeričnimi pristopi v analizi 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.

#### **Objectives and Competences:**

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:**

<p><u>Znanje in razumevanje</u> 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.</p>	<p><u>Knowledge and Comprehension</u> 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.</p>
<p><u>Uporaba</u> Študent pridobi znanja za uporabo na področju kemijskih raziskav ter na področju raziskav materialov in bioloških snovi.</p>	<p><u>Application</u> Student acquires practical knowledge to use in chemical research and research of materials and biological samples.</p>
<p><u>Refleksija</u> Poveže konkretno uporabo določene kemijsko-fizikalne zakonitosti z rezultati, ki jih pridobi z meritvami.</p>	<p><u>Analysis</u> Student connects the application of a certain physico-chemical principle with the results obtained by the measurement.</p>
<p><u>Prenosljive spretnosti</u> Osvoji metodologijo in raziskovalne pristope, obvlada problemsko orientirane raziskave, zna uporabljati strokovno in znanstveno literaturo in obvlada veščine poročanja in obravnave podatkov.</p>	<p><u>Skill-transference Ability</u> 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.</p>

**Metode poučevanja in učenja:**

Predavanja in seminarska dela iz aktualne tematike, demonstracijske vaje

**Learning and Teaching Methods:**

Lectures, seminar coursework on realistic problems, demonstrative laboratory work

**Načini ocenjevanja:**

Pisni in ustni izpit:  
ocene od 6-10 (poz.) oz. 1-5 (neg.).  
Seminarska naloga.  
Laboratorijske vaje.

Delež (v %) /

Weight (in %) **Assessment:**

<p>Pisni in ustni izpit: ocene od 6-10 (poz.) oz. 1-5 (neg.). Seminarska naloga. Laboratorijske vaje.</p>	<p><b>60 %</b> <b>30 %</b> <b>10 %</b></p>	<p>Written and oral exam: grades 6-10 (pass) or 1-5 (fail). Seminar coursework. Laboratory work.</p>
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Opravljene vaje in seminarska naloga so pogoj za pristop k izpitu.		Finished laboratory and seminar work are prerequisites for the exam.
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**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>sub</sub>-symmetric fullerenehexamalononic acid C<sub>sub</sub>(66)(COOH)<sub>sub</sub>(12) by ion-chromatography and capillary electrophoresis. *J. chromatogr. A* 2007, 1169, 86-94.

**UČNI NAČRT PREDMETA / COURSE SYLLABUS**

<b>Predmet:</b>	ORGANOKOVINSKA IN SUPRAMOLEKULARNA KEMIJA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

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:

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

Prerequisites:

The course has to be assigned to the student.

Vsebina:

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

Content (Syllabus outline):

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

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

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.

**Intended Learning Outcomes:**Knowledge and Comprehension

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



<p>Pridobitev znanj s področja dela v inertni atmosferi in vakuumu.</p>	<p>ds. Acquire knowledge of the principles of catalytic processes and understanding the role of metals and ligands. Acquire a practical skills for working in an inert atmosphere and vacuum.</p>
<p><u>Uporaba</u> 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, ...).</p>	<p><u>Application</u> Acquired knowledge and skills can be used to solve practical scientific problems and discuss about them. Using modern knowledge and methods of organometallic and supramolecular chemistry in other areas (chemistry reagents, stereochemistry, materials chemistry, nanotechnology, biological chemistry, pharmacy, medicine...).</p>
<p><u>Refleksija</u> 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 sintezni 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.</p>	<p><u>Analysis</u> 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.</p>
<p><u>Prenosljive spretnosti</u> 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.</p>	<p><u>Skill-transference Ability</u> 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.</p>

**Metode poučevanja in učenja:**

Predavanje in vaje.

**Learning and Teaching Methods:**

Lectures and laboratory work.

Delež (v %) /

**Načini ocenjevanja:**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  $\beta$ -keto amides and  $\beta$ -enamino carboxamides, *Tetrahedron* **2007**, *63*, 10902–10913.
- A. Pevec, F. Perdih, J. Košmrlj, B. Modec, H. W. Roesky, A. Demšar: Lithium complexes with a  $[\text{Cp}^*_2\text{Ti}_2\text{F}_7]^-$  ligand:  $^{19}\text{F}$  NMR probe for lithium solvation.- *Dalton Trans.* **2003**, 420-425.
- A. Pevec: Syntheses and Solid-State and Solution Structures of  $[\text{Ba}\{(\text{C}_5\text{Me}_5)_2\text{Ti}_2\text{F}_7\}_2(\text{hmpa})]$  and  $[\text{Ba}_8\text{Ti}_6\text{F}_{30}\text{I}_2(\text{C}_5\text{Me}_5)_6(\text{hmpa})_6][\text{I}_3]_2$ . - *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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

**Vrsta predmeta / Course Type:**

obvezni / Mandatory

**Univerzitetna koda predmeta / University Course Code:**

KE213

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

**Nosilec predmeta / Lecturer:**

prof. dr. Andrej Petrič / Dr. Andrej Petrič, 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:**

**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<sub>a</sub>, uporaba podatkov o pK<sub>a</sub> pri ravnotežjih in reakcijah. Reakcijska hitrost, red reakcije, uporaba podatkov o reakcijski kinetiki pri predlaganju mehanizma reakcije, Arrheniusova enčba, aktivacijska energija, primarni kinetski izotopski efekt.

**3. Prehodno stanje.**

**Content (Syllabus outline):**

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, pK<sub>a</sub>, 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, Hammond postulate, solvent effects,

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 ( ) 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.

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*. (2<sup>nd</sup> 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:**Znanje in razumevanje

Poznavanje poteka osnovnih organskih reakcij in metod za študij oziroma dokazovanje reakcijskih mehanizmov. Razumevanje in poznavanje vplivov na potek kemijskih reakcij.

Uporaba

Razvita sposobnost študenta, da pridobljeno znanje uporabi za raziskavo mehanizma neznane reakcije.

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.

Prenosljive spretnosti

Pri predmetu se študenti z reševanjem znanih in neznanih problemov izurijo v uporabi znanja, analitičnega mišljenja in uporabe literaturnih virov.

**Intended Learning Outcomes:**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.

Application

Student will be able to apply the acquired knowledge in reaction mechanism investigation.

Analysis

Being aware that chemical reactions never follow exclusively one elementary mechanism and that for complete analysis every reaction requires thorough investigation.

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:**

- Predavanja in vaje.

**Learning and Teaching Methods:**

Lectures and practical laboratory work.

**Načini ocenjevanja:**

6 testov in pisni izpit. Na osnovi seštevka točk petih najbolje ocenjenih testov (do 5x10 točk), in končnega izpita (do 350), skupaj maksimalno 400 bo določena končna ocena. Način določanja končne ocene na osnovi zbranega števila točk bo določen v vsakoletnem izvedbenemu načrtu predmeta.  
10 (odlično), 9 in 8 (prav dobro), 7 (dobro), 6 (zadostno), 1-5 (nezadostno)

Delež (v %) /

Weight (in %) /

**Assessment:**

6 tests and written exam.

**Reference nosilca / Lecturer's references:**

- KOŽELJ, Matjaž, PETRIČ, Andrej: Strong-acids-promoted protiodeacylation of sterically nonhindered alkyl aryl ketones. *Synlett* **2007**, 1699-1702.  
- ČEH, Simon, PETRIČ, Andrej: A variety of products from a "simple" reaction of [1-(6-acetyl-2-naphthyl)piperidin-4-yl]methyl 4-methylbenzenesulfonate with nucleophiles in DMF-K<sub>2</sub>CO<sub>3</sub>. *J. Chem. Soc., Perkin trans., I* **2000**, 359-362.

- ŽABJEK, Alenka, PETRIČ, Andrej: A general method for the alkaline cleavage of enolisable ketones. *Tetrahedron Lett.* **1999**, *40*, 6077-6078.

UL  
EFKKT

**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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	4 <sup>th</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

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

**Content (Syllabus outline):**

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

- praktična aplikacija metode razvoja novih 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 its 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 Creativity 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:**

#### 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

#### 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).

#### Refleksija

Študent bo interpretiral ter pred kolegi analiziral lastno razumevanje vsebine aktualnih člankov in razpoznavanja trendov. V skupinskem delu študentje analizirajo delo

### **Intended Learning Outcomes:**

#### 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

#### 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.).

#### 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

<p>svoje in ostalih skupin in podajajo konstruktivno kritiko.</p>	<p>own work and work of other groups and give constructive feedback.</p>
<p><b>Prenosljive spretnosti</b> 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.</p>	<p><b>Skill-transference Ability</b> 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.</p>

**Metode poučevanja in učenja:**

<p>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 sprotnege 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</p>
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**Learning and Teaching Methods:**

<p>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</p>
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Delež (v %) /

**Načini ocenjevanja:**

Weight (in %) **Assessment:**

<p>Redna poročila o napredku</p>	<p><b>20</b></p>	<p>Regular progress reports</p>
<p>Končno poročilo in predstavitev o rešitvi problema</p>	<p><b>40</b></p>	<p>Final report and presentation on the solution of the problem</p>
<p>Domače naloge, sodelovanje na srečanjih</p>	<p><b>20</b></p>	<p>Homeworks and active participation in sessions</p>
<p>Izpit pisni in/ali ustni.</p>	<p><b>20</b></p>	<p>Written and / or oral exam. Grades 6-10.</p>
<p>Ocene: 6-10 pozitivno</p>		

**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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1st and 2 <sup>nd</sup>

**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:**

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Raziskovalno delo se opravlja na področju kemije. Vsebina in naslov se določata v soglasju z izbranim mentorjem – nosilcem ene izmed vsebin v programu.

**Content (Syllabus outline):**

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 raziskovalnem 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:**

##### 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.

##### Uporaba

Znanje in pridobljene veščine bo študent lahko uporabil pri opravljanju poklica in opravljanju magistrskega dela.

##### Refleksija

Povezovanje vseh pridobljenih teoretičnih znanj z reševanjem problemov na področju kemije ter kritični pogled na uporabnost teh znanj.

#### **Intended Learning Outcomes:**

##### 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.

##### Application

Acquired knowledge is necessary for Master's thesis work and for professional work.

##### Analysis

Integration of knowledge from different topics of chemistry and supporting sciences; Development of a critical view on the knowledge applicability.

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

- Individualno delo mentorja in samostojno študijsko in raziskovalno delo.

**Learning and Teaching Methods:**

Independent research work supervised by the mentor.

**Načini ocenjevanja:**

Oddano poročilo o delu in ustna predstavitev poročila na seminarju. Oboje oceni mentor.

Ocena: opravil/ni opravil.

Delež (v %) /

Weight (in %) **Assessment:**

pass/fail

**Reference nosilca / Lecturer's references:**

/

**UČNI NAČRT PREDMETA / COURSE SYLLABUS**

<b>Predmet:</b>	SODOBNI ANORGANSKI MATERIALI IN KATALIZATORJI
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	2 <sup>nd</sup>

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

Prerequisites:

The course has to be assigned to the student.

Vsebina:

**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

Content (Syllabus outline):

**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's 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:

**Cilji:** Poglobljeno spoznavanje določenih tipov sodobnih anorganskih materialov in katalizatorjev, sinteznih tehnik in raznovrstnih metod za njihovo karakterizacijo.

**Kompetence:** Izpeljava celotnega projekta: sinteza in karakterizacije tako katalizatorja kot anorganskega materiala, vključno z literaturnim pregledom in načrtovanjem.

### Objectives and Competences:

**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:

#### 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 praktičnega znanja z izvedbo dveh različnih projektnih nalog: sinteza in karakterizacija novega materiala ter sinteza in karakterizacija katalizatorja.

#### 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 odročja materialov.

#### 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.

#### Prenosljive spretnosti

Študent zna uporabljati zbirke podatkov, izbrati najbolj primerne sintezne postopke za

### Intended Learning Outcomes:

#### 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.

#### Application

Integration of acquired knowledge and planning modifying 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.

#### 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.

#### 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:**

- predavanja
- seminar
- izpeljava projektne naloge

**Learning and Teaching Methods:**

- Lectures
- Seminars
- Execution of one project

Delež (v %) /

Weight (in %) **Assessment:**

**Načini ocenjevanja:**

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:**

- R. Cerc Korošec, P. Bukovec, B. Pihlar, A. Šurca Vuk, B. Orel, G. Dražić: Preparation and structural investigations of electrochromic nanosized NiO<sub>x</sub> films made via the sol-gel route. - *Solid state ion.* **2003**, *165*, 191-200.
- J. Moškon, R. Dominko, M. Gaberšček, R. Cerc Korošec, J. Jamnik. Citrate-derived carbon nanocoatings for poorly conducting cathode. - *J. Electrochem. Soc.* **2006**, *153*, A1805-A1811.
- P. Umek, R. Cerc Korošec, B. Jančar, R. Dominko, D. Arčon: The Influence of the Reaction Temperature on the Morphology of Sodium Titanate 1D Nanostructures and a Study of Their Thermal Stability. - *J. nanosci. nanotechnol.* **2007**, *9*, 3502-3508.

<b>UČNI NAČRT PREDMETA / COURSE SYLLABUS</b>	
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<b>Predmet:</b>	SPEKTROKEMIJSKA ANALIZA
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	3 <sup>rd</sup>

<b>Vrsta predmeta / Course Type:</b>	izbirni strokovni / Elective Professional
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<b>Univerzitetna koda predmeta / University Course Code:</b>	K2I12
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Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	30	15 LV	/	/	75	5

<b>Nosilec predmeta / Lecturer:</b>	prof. dr. Marjan Veber / Dr. Marjan Veber, Full Professor
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<b>Jeziki / Languages:</b>	<b>Predavanja / Lectures:</b> slovenski / Slovenian
	<b>Vaje / Tutorial:</b> /

<b>Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:</b>	<b>Prerequisites:</b>
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	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.

**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**

**Novejši vidiki atomske absorpcijske spektrometrije**- 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 standardizacije.

**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.

**spectroscopy**; theoretical aspects and its role in separation and preconcentration procedures.

**New concepts of atomic absorption spectrometry**; high resolution continuum source AAS.

**Characteristics of high temperature sources in spectrometry** - inductively coupled plasma (ICP), 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. Golightly: 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:

*Cilji:* Študenti spoznajo teoretske osnove sodobnih spektroskopskih metod.  
*Kompetence:* Pridobijo nekatere praktične izkušnje za delo z zahtevno instrumentacijo.

#### Objectives and Competences:

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:

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

**Metode poučevanja in učenja:**

Predavanja, seminarji, laboratorijske vaje.

**Learning and Teaching Methods:**

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, Report on practical work,
Pisno poročilo o eksperimentalnem delu, Ustni izpit	10%	
	50%	Oral examination

**Reference nosilca / Lecturer's references:**

1. J.A. Koropchak, M. Veber, Thermospray Sample Introduction to Atomic Spectrometry; Critical Reviews in Analytical Chemistry, 23(3), (1992), 113-141.
2. P. Razpotnik, M. Veber, Investigations into nonspectroscopic effects of organic compounds in inductively coupled plasma mass spectrometry, *Acta chim. slov.*, 2003, vol 50, No. 4, 633-644.
3. M. Kovačević, W. Goessler, N. Mikac, M. Veber, Matrix effects during phosphorus determination with quadrupole inductively coupled plasma mass spectrometry. *Anal. bioanal. chem.*, 2005, vol. 383, no. 1, 145-151.

**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, 2 <sup>nd</sup> Cycle	/	2 <sup>nd</sup>	4 <sup>th</sup>

**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:**Študent oz. kandidat mora imeti predmet  
opredeljen kot študijsko obveznost.**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

- 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).
- Teoretske osnove termičnega razpada trdnih snovi; bazna linija pri TG in DSC krivulji.
- Temperaturna kalibracija termoanalizatorja, kalibracija DSC instrumenta; fleksibilna kalibracija.
- Analiza eksperimentalnih podatkov izmerjenih TG in DSC krivulj vzorcev z znano sestavo, primerjava z

**Content (Syllabus outline):**

- 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).
- Thermal decomposition of solids (theoretical principles), baseline of TG and DSC curve.
- Temperature calibration thermoanalyser, calibration of a DSC instrument, flexible calibration.
- 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

<p>prebrati in komentirati rezultat). S pomočjo literature se nauči termično analizo uporabiti za reševanje kompleksnih problemov.</p>	<p>(performing measurement, interpret and comment a result). Thermal analysis can be used for solving more complex issues with the aid of references.</p>
<p><u>Uporaba</u> 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.</p>	<p><u>Application</u> 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.</p>
<p><u>Refleksija</u> 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.</p>	<p><u>Analysis</u> 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.</p>
<p><u>Prenosljive spretnosti</u> 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.</p>	<p><u>Skill-transference Ability</u> 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.</p>

**Metode poučevanja in učenja:**

- Predavanje
  - problemsko delo na seminarjih
  - laboratorijske vaje: meritve
- Priprava, izvedba in predstavitev projekta

**Learning and Teaching Methods:**

- Lectures
- Coursework during seminars
- Laboratory practice: measurements
- Project preparation and presentation

**Načini ocenjevanja:**

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



- pisno poročilo - ocena projektne naloge s predstavitvijo in odgovori na vprašanja	50 %  50 %	-written report -project
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**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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

izr. prof. dr. Jurij Reščič / Dr. Jurij Reščič, Associate Professor

**Jeziki / Languages:**

**Predavanja / Lectures:** slovenski / Slovenian

**Vaje / Tutorial:** slovenski / Slovenian

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

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

**Prerequisites:**

The course has to be assigned to the student.

**Vsebina:**

Ponovitev in obravnava matematičnih orodij na splošno s poudarkom na konkretnih numeričnih primerih s področja kemije.

Uporaba nekaterih splošno uporabljenih 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 (Fortran ali C).

Razčlenitev problema, prikaz poteka reševanja z blokovno shemo, opis in razlaga izbranega

**Content (Syllabus outline):**

Introduction into known 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 (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.

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 (Gaussova metoda eliminacije, Cramerjevo pravilo). Matrike, inverzija matrik, lastni vektorji in lastne vrednosti matrik, reševanje nelinearnih enačb (metoda bisekcije, Newton-Raphsonova metoda) 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, avtokorelacija.

Main topics: rounding errors, statistical analysis (mean value, standard deviation), linear regression analysis and correlation coefficients, recursion formulae, interpolation, systems of linear equations, matrices, inversion of matrices, eigenvectors and eigenvalues, solving nonlinear equations (bisection, Newton-Raphson's method), 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 1<sup>st</sup> and 2<sup>nd</sup> 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:

- Z. Bohte, Numerične metode, DZS, Ljubljana 1978. (20%)
- John H. Mathews, Kurtis D. Fink, Numerical methods using MATLAB 4<sup>th</sup> ed., Prentice Hall, 2004. (10%)
- K. J. Johnson, Numerical Methods in Chemistry, Dekker, New York 1980. (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 2<sup>nd</sup> ed., Wiley, New York 2001. (10%)
- Priročniki za izbrani programski jezik

#### Cilji in kompetence:

*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 programiranja v enem izmed višjenivojskih

#### Objectives and Competences:

*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 analysis and high-performance computing.

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.

Usage of common software to present and interpret experimental data.

**Predvideni študijski rezultati:**

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.

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.

Refleksija

Študent pridobi občutek, da se je sposoben lotiti poljubnega numeričnega problema, za katerega še ni (ali pa ne pozna) napisanega računalniškega programa.

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.

**Intended Learning Outcomes:**

Knowledge and Comprehension

The subject is aimed toward basic numerical methods commonly used throughout various natural sciences and especially in chemistry. A student learns to identify the problem, dissect it, and solve it using a self-developer computer program or algorithm.

Application

The acquired knowledge is widely applicable and is not only chemistry-related. A student is able to solve problems encountered during the study and later, independent on the field of science.

Analysis

A student becomes confident about her/his ability to solve a given numerical problem using a computer program developer on her/his own.

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:**

- Predavanja.
- Praktične vaje na računalniku.

**Learning and Teaching Methods:**

Lectures and computer lab course.

**Načini ocenjevanja:**

Delež (v %) /

Weight (in %) **Assessment:**

Seminarska naloga in pisni izpit. Ocene: 6-10 (pozitivno), 1-5 (negativno) ob upoštevanju Statuta UL in fakultetnih pravil.		Seminar, written exam.
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**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**

<b>Predmet:</b>	VODE KOT HIDROGEOLOŠKI, EKOLOŠKI IN ANALIZNI SISTEM
<b>Course Title:</b>	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, 2 <sup>nd</sup> Cycle	/	1 <sup>st</sup>	1 <sup>st</sup>

**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:**

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

**Prerequisites:**

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

<p>-interpretacija rezultatov</p> <p><b>IZBIRA SPREMENLJIVK KAKOVOSTI VOD</b></p> <p>-hidrološke spremenljivke</p> <p>-splošne spremenljivke</p> <p>-hranilne snovi</p> <p>-organska snov</p> <p>-prevladujoči ioni</p> <p>-druge anorganske spremenljivke</p> <p>-kovine</p> <p>-organski kontaminanti</p> <p>-mikrobiološki indikatorji</p> <p>-izbira spremenljivk</p> <p><b>PODTALNICA</b></p> <p>- značilnosti vodonosnikov</p> <p>- interakcije voda-prst-kamnina</p> <p>- vidiki kakovosti podtalnice</p> <p>- strategije ocenjevanja kakovosti</p> <p>- primeri ocenjevanj kakovosti podtalnice</p> <p><b>REKE</b></p> <p>-hidrološke značilnosti</p> <p>-kemijske značilnosti</p> <p>-biološke značilnosti</p> <p>-najpomembnejši vidiki kakovosti rek</p> <p>-strategije ocenjevanja kakovosti rečnih sistemov</p> <p>-pristopi k spremljanju in ocenjevanju kakovosti rečnih sistemov – študij primerov</p> <p><b>JEZERA</b></p> <p>-značilnosti in tipologija</p> <p>-vidiki kakovosti</p> <p>-strategije ocenjevanja kakovosti jezer</p> <p>-pristopi k ocenjevanju jezer – študij primerov</p> <p><b>ANALIZA IN INTERPRETACIJA PODATKOV O KAKOVOSTI VOD</b></p> <p>-Preverjanje zanesljivosti podatkov (anionsko-kationska bilanca, različna preverjanja, relativni odnosi med ioni)</p> <p>-Sklepanje na kamninski izvor</p> <p>-Grafične metode (»Stiff« diagram, Piper diagram)</p> <p>-Prepoznavanje reakcij v podtalnici</p>	<ul style="list-style-type: none"> <li>- data quality control</li> <li>- interpretation</li> </ul> <p><b>SELECTION OF WATER QUALITY VARIABLES</b></p> <ul style="list-style-type: none"> <li>- hydrological variables</li> <li>- general variables</li> <li>- nutrients</li> <li>- organic matter</li> <li>- major ions</li> <li>- other inorganic variables</li> <li>- metals</li> <li>- organic contaminants</li> <li>- microbiological indicators</li> <li>- selection of variables</li> </ul> <p><b>GROUNDWATER</b></p> <ul style="list-style-type: none"> <li>- characteristics of groundwater bodies</li> <li>- water-soil-rock interactions</li> <li>- ground water quality issues</li> <li>- assessment strategies</li> <li>- examples of ground water assessment</li> </ul> <p><b>RIVERS</b></p> <ul style="list-style-type: none"> <li>- hydrological characteristics</li> <li>- chemical characteristics</li> <li>- biological characteristics</li> <li>- major water quality issues in rivers</li> <li>- strategies for water quality assessment in river systems</li> <li>- approaches to river monitoring and assessment: case studies</li> </ul> <p><b>LAKES</b></p> <ul style="list-style-type: none"> <li>- characteristics and typology</li> <li>- water quality issues</li> <li>- assessment strategies</li> <li>- approaches to lake assessment: case studies</li> </ul> <p><b>ANALYSIS AND INTERPRETATION OF WATER QUALITY DATA</b></p> <ul style="list-style-type: none"> <li>- reliability of data (anion-cation balance, miscellaneous checks, relative amounts of ions reported)</li> <li>- source-rock deduction</li> <li>- graphical methods – “Stiff” diagram, Piper diagram</li> <li>- ground water reactions</li> </ul>
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**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:**

*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 and Competences:**

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:**

Znanje in razumevanje

Študent zna spremljati in ocenjevati kakovost različnih vodnih virov.

Uporaba

Uporaba pridobljenih rezultatov za suveren nadzor nad kakovostjo vodnih virov.

Refleksija

Študent ima kritičen odnos do kakovosti vodnih virov.

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

**Intended Learning Outcomes:**

Knowledge and Comprehension

Student develops knowledge and comprehension necessary for monitoring and evaluation of water quality of different water bodies.

Application

Student develops ability of using analytical data for water quality evaluation.

Analysis

Student adopts critical attitude towards quality of different water bodies.

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 seminarскими nalogami (za doseganje višje analizne učinkovitosti in razvijanje osebne odgovornosti in odgovornosti do skupine študentje celotno skupino vzorcev vod analizirajo timsko z delitvijo posamezni zadolžitve). Skupinsko in individualno vrednotenje analiznih rezultatov. Pisanje seminarske naloge, interpretacija rezultatov v povezavi s postavljenimi 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.

Delež (v %) /

Weight (in %) **Assessment:**

**Načini ocenjevanja:**

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.