

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet: IZBRANA POGLAVJA IZ ANORGANSKE KEMIJE
Course Title: SELECTED TOPICS IN INORGANIC CHEMISTRY

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
DR Kemijske znanosti, 3. stopnja	/	1.	1. in 2.
Doctoral programme in Chemical Sciences, 3 rd Cycle	/	1 st	1 st and 2 nd

Vrsta predmeta / Course Type: izbirni/Elective

Univerzitetna koda predmeta / University Course Code: KZ301

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

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

Študent s soglasjem mentorja med spodaj navedenimi temami izbere tiste, ki so najtesneje povezane z njegovim raziskovalnim delom. Nosilec predmeta in vodja študija poskrbita, da obseg študentovega dela ustreza 5 KT. Če je izvajalcev več, izvajanje koordinira nosilec.

Priprava in uporaba spojin kovinskih elementov:

Priprava spojin elementov, ki imajo praktične aplikacije. Sistematičen pregled sinteznih principov za pripravo spojin in metod njihove karakterizacije.

Poglobljen pregled izbranih primerov sodobnih uporab: modelne koordinacijske spojine

Content (Syllabus outline):

From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

Preparation of compounds with practical use.

Systematic review of synthetic principles used for the preparation of compounds and methods for their characterization.

In-depth review of selected, up-to-date examples of practical applications: metal

(zaščita lesa; modeli encimov, ipd.), fotosenzitivne rutenijeve spojine v Graetzlovih celicah, fluorescenčne kovinske spojine in uporaba v analitiki, spojine zlata in nanotehnologija, elektrodni materiali. Pregled nekaterih najuspešnejših kovinskih katalizatorjev, ki se uporabljajo tudi v industriji (Noyori, Grubbs, Heck, itd.). Mehanizmi delovanja.

Biološko aktivni kompleksi. Pregled nekaterih spojin ki imajo dokazano biološko aktivnost in so že v klinični rabi ali pa v preizkusni fazi. Načrtovanje in sinteza novih biološko aktivnih koordinacijskih spojin, ki temeljijo na poznavanju mehanizma delovanje že obstoječih učinkovin, oziroma na podlagi najnovejših spoznanj o delovanju posameznih bioloških sistemov. Pri tem bodo uporabljene najnoveše strategije in metode. Pomembni vidiki tega načrtovanja so oblika/ struktura ter fiziološka dostopnost učinkovin, glede na njeno ciljno uporabo. Pri tem študent pridobi znanje, ki mu omogoča samostojno delo na področju biološko aktivnih spojin.

Kovinski kompleksi z makromolekulami. Kovinski kompleksi z nekaterimi makromolekulami imajo velik aplikativni pomen. V splošnem ločimo dva sintezna pristopa k pripravi teh spojin. Pri prvi metodologiji gre za koordinacijo kovinskega kompleksa na že formiran polimer, pri drugi pa enostaven kovinski kompleks reagira z monomerno enoto in v reakciji polimerizacije nastane makromolekula, ki ima kovinski atom pogosto v osnovni polimerni verigi. Sintezne poti za pripravo kovinskih kompleksov z makromolekulami, strukturne značilnosti in tipične lastnosti teh kompleksov, biomedicinske aplikacije.

Organokovinske spojine. Načrtovanje sinteze organokovinskih spojin, eksperimentalne tehnike pri sintezi, karakterizacija produkta. Dinamična NMR spektroskopija kot metoda za študij fluksionalnih organokovinskih in drugih molekul: osnove, določanje termodinamskih in kinetičnih parametrov in mehanizma dinamičnega procesa. Uporaba dinamične

complexes as model compounds (wood preservation; enzyme models, etc.), photosensitive ruthenium compounds used in Graetzel cells, fluorescence metal compounds and their application in analytics, gold compounds and nanotechnology, electrode materials.

Review of some most successful metal catalyst also used in industrial processes (Noyori, Grubbs, Heck, etc.). Mechanisms of action.

Biologically active complexes. Review of selected compounds with confirmed biological activity already in clinical use, or have entered clinical trials. Design and synthesis of novel biologically active coordination compounds. Design will be based on the knowledge derived from the approved drugs (with known mechanisms of action) or from modern principles about functioning of biological systems. Novel strategies and methods will be used in the process. Through these procedures the student will acquire the knowledge for independent work in the field of biologically active compounds.

Metal complexes with macromolecules. Metal complexes with macromolecules have great potentials for application. In general, two approaches for the synthesis of macromolecular metal complexes are known:

- coordination of metal ions on bulk polymers
- preparation of a metal complex with monomeric unit followed by polymerization and formation of a polymer with metal ion bonded to the polymeric chain. Synthesis of metal complexes with macromolecules, characterization and structural properties of the macromolecular metal complexes, applications in biomedicine.

Organometallic compounds. Planning of the syntheses of organometallic compounds, experimental techniques of the syntheses, characterization of the products. Dynamic NMR spectroscopy as a tool for the study of dynamic behaviour of molecules: background, determination of thermodynamic and kinetic parameters and mechanism of dynamic process. The use of dynamic NMR spectroscopy

NMR spektroskopije za proučevanja mehanizma reakcij, kataliziranih z organokovinskimi katalizatorji.

Kovine v okolju. Razporeditev kovin in kovinskih spojin v okolju, esencialni in toksični elementi, naravni in antropogeni izvori, pomen kovin za žive organizme. Reakcije in kroženje kovin in kovinskih spojin v okolju (topnost spojin, ligandi v okolju, nastanek koordinacijskih spojin, reakcije koordinacijskih spojin, stabilnost koordinacijskih spojin, obarjanje, adsorpcija, kemisorpcija, ionska izmenjava, redoks reakcije, frakcionacija kovin v tleh). Obremenitev okolja s kovinskimi spojinami (toksičnost, mejne vrednosti, zakonodaja). Povezovanje navedenih vsebine z aktualnimi okoljskimi problemi. Sanacija tal in vode, stabilizacija odpadkov (ocena stanja pri onesnaženju s kovinami, principi sanacije, izbira metode sanacije).

for studying the reaction mechanism catalyzed by organometallic catalysts.

Metals in the environment. Distribution of metals and their compounds in the environment, essential and toxic metal compounds, geochemical and anthropogenic sources of metals, importance of metals for living beings. Reactions and circulation of metals in environment (solubility of metal compounds; ligands for metals in the environment; origin, reactions and stability of coordination compounds; precipitation, adsorption, chemisorption, ionic exchange, redox reaction and fractionation of metals in ecosystems). Pollution of the environment with metal compounds (toxicity, limit values, legislation). Connection of mentioned topics with actual environmental problems. Remediation of soil and water, stabilisation of wastes (evaluation of the state of contamination with metals, principles and suitable methods of rehabilitation).

Temeljna literatura in viri / Readings:

Literaturo določijo izvajalci glede na izbrane vsebine, za primeren skupni obseg (cca. 300 do 400 strani) poskrbi nosilec./ Literature will be determined by lecturers according to selected topics, while course coordinator will take care for obtaining suitable total volume (cca. 300 and 400 pages).

- C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th Edition, Pearson Education Limited, Harlow, England, 2018 (1251 strani – izbrana poglavja).
- H.-B. Kraatz, N. Metzler-Nolte (Eds.) Concepts and models in bioinorganic chemistry, Third Edition, Wiley-VCH, Weinheim, Germany, 2006 (443 strani- izbrana poglavja).
- B. A. Richardson, in Wood preservation, Second Edition, Preservation Chemicals, E. & F.N. Spon, London, England, 97-152 (2002).
- D. B. Mitzi, Solution processing of inorganic materials, Hoboken Wiley, New Jersey, 2009 (497 strani - izbrana poglavja).
- K. Kalyanasundaram, Dye-sensitized solar cells, CRC Press, Lausanne, 2010 (604 strani - izbrana poglavja).
- P. Day P., Molecules into materials, World Scientific, New Jersey, 2007 (586 strani - izbrana poglavja).
- E. Alessio (Ed.), Bioinorganic Medicinal Chemistry. Wiley-VCH Verlag & Co. KGaA: Weinheim, Germany, 2011 (422 strani- izbrana poglavja).
- A. Sigel, H. Sigel (Eds.), Metal ions in biological systems, vol. 1-44, Marcel Dekker, Inc., New York, Basel 2004 (izbrana poglavja).
- A. S. Abd-El-Aziz et al (Eds.) Macromolecules containing metal and metal-like elements, Vol.3, Biomedical applications, Hoboken Wiley, New Jersey 2004 (208 strani).

- C. Elschenbroich, A. Salzer, Organometallics, A Concise Introduction, Third Edition, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2006 (818 strani).
- J. P. Vernet, Heavy metals in the environment, Elsevier Science, 1991 (424 strani - izbrana poglavja).
-Novejši pregledni članki iz revij.

Cilji in kompetence:

Študent pridobi poglobljeno znanje o izbranih poglavjih anorganske kemije. Spozna strategije načrtovanja sintez ter se nauči iskati in interpretirati povezave med zgradbo, lastnostmi in potencialno uporabnostjo izbranih vrst spojin. Nauči se uporabljati različne eksperimentalne metode pri razreševanju problemov, povezanih z izbranimi vrstami spojin.

Objectives and Competences:

Student acquires knowledge on selected chapters in inorganic chemistry, knows how to plan strategies for syntheses and is able to interpret the relationships between the structure, properties and potential application of selected types of compounds; knows how to apply various experimental methods to resolve problems associated with selected types of compounds.

Predvideni študijski rezultati:

Znanje in razumevanje

Predmet s poglobljenim pregledom izbranih poglavij iz anorganske kemije, predstavlja nadaljevanje anorganskih predmetov iz nižjih nivojev študija. Študent je sposoben demonstrirati znanje in razumevanje bistvenih podatkov, konceptov in teorij, ki so povezane z izbranimi pojmi vsebovanimi v opisu vsebine predmeta.

Uporaba

Študent spozna, kako znanje o raznih elementih periodnega sistema uporabiti za načrtovanje sintez spojin in tudi predvidevanje njihovih lastnosti. Sposoben naj bi bil uporabljati svoje znanje interdisciplinarno in na praktičnih primerih. Študent pridobi izkušnje kako narediti analizo podatkov v določenem sistemu povezanem z anorgansko kemijo. Spozna različne uporabe anorganskih elementov, spojin in materialov.

Refleksija

Študent za izbrano temo pripravi seminar na osnovi lastnega razumevanja vsebine člankov iz strokovnih revij oziroma poglavij iz knjig. Pri pripravi gradiva uporablja refleksijo, pri čemer sistematično in ustvarjalno razmišlja, da bi bolje razumel procese ter na ta način izboljšuje prihodnja ravnanja. V seminarju

Intended Learning Outcomes:

Knowledge and Comprehension

This course represents a deeper insight into selected chapters in inorganic chemistry and is a continuation of inorganic courses from lower levels of study. The student is able to demonstrate the knowledge and understanding of the essential data, concepts and theories related to the selected content of the course described above.

Application

Student learns how knowledge about various elements of the periodic table is used for the rational synthesis of compounds as well as to anticipate their properties. The emphasis is on the interdisciplinary application of his/her knowledge and on problem-based examples. Student acquires knowledge to analyse data in certain inorganic chemistry system and learns about versatile uses of inorganic elements, compounds and materials.

Analysis

Student will prepare a seminar on the chosen topic. This will be based on an in-depth analysis of the topic on the basis of his own understanding of the content of articles in scientific journals or book chapters. Systematic and creative thinking should be used to better understand the processes and to improve her/his future actions. In seminar selected topic

izbrano temo predstavi in analizira podatke ter predstavi tudi svoj pogled na tematiko. Temo predstavi tudi pred kolegi.

is presented, analysed and also her/his own view should be given. The topic is presented also to student colleagues.

Prenosljive spretnosti

Poznavanje vsebin in način dela omogočata boljše razumevanje zakonitosti tudi pri drugih predmetih študija in povečata širino znanja. Samostojno delo (iskanje literature, zbiranje in interpretacija podatkov, predstavitve) je prenosljivo na mnoge druge predmete študija in pa seveda tudi na kasnejše življenjske situacije. Naučene spretnosti so kot podlaga koristne tudi pri praktičnem delu in izdelavi teze, prav tako pa služijo tudi pri osebnem profesionalnem razvoju.

Skill-transference Ability

The knowledge and skills obtained during this course also enable better understanding of the principles in other courses of doctoral study and broaden the scientific knowledge. Individual work (literature search, collection and interpretation of data, presentation) is transferable to many other subjects of study and definitely also to many real situations in life. Learned skills are useful as a basis for practical work during preparation of the thesis and also help in their personal professional development.

Metode poučevanja in učenja:

Konzultacije za izbiro najprimernejše teme. Samostojno iskanje literaturnih virov ter obdelava in interpretacija podatkov. Priprava in predstavitve seminarske teme.

Learning and Teaching Methods:

Consultations to select the most appropriate topic. Autonomous literature search, processing and interpretation of data. Preparation and public project presentation.

Delež (v %) /

Načini ocenjevanja:

Weight (in %) **Assessment:**

Priprava in predstavitve seminarske naloge (80 %) in njen ustni zagovor (20 %).

Preparation and presentation of seminar (80 %) and oral exam (20 %).

Reference nosilca / Lecturer's references:

J. Kladnik, A. Dolinar, J. Kljun, D. Perea, J. Grau-Expósito, M. Genescà, M. Novinec, M. J. Buzon*, I. Turel*, Zinc pyrithione is a potent inhibitor of PLPro and cathepsin L enzymes with ex vivo inhibition of SARS-CoV-2 entry and replication, *J. Enzyme Inhib. Med. Chem.*, **37**:1, 2158-2168 (2022).

J. Kladnik, J. P. C. Coverdale, J. Kljun, H. Burmeister, P. Lippman, F. G. Ellis, A. M. Jones, I. Ott, I. Romero-Canelón*, and I. Turel*, Organoruthenium Complexes with Benzo-fused Pyrithiones Overcome Platinum Resistance in Ovarian Cancer Cells, *Cancers*, **13**, 2493 (2021).

A. Mitrović, J. Kljun, I. Sosič, M. Uršič, A. Meden, S. Gobec, J. Kos, I. Turel, Nitroxoline-ruthenium complexes impair tumor cell invasion at non-cytotoxic concentrations by inhibition of cathepsin B activity, *Inorg. Chem.*, **58**, 12334–12347 (2019).

S. Seršen, J. Kljun, F. Požgan, B. Štefane, I. Turel, Novel organoruthenium(II) β -diketonates as catalysts for ortho-arylation via C–H activation, *Organometallics*, **32**, 609–616 (2013).