

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 nd Cycle	/	1 st	2 nd

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
izr. prof. dr. Janez Cerar / Dr. Janez Cerar, Associate Professor
prof. dr. Matija Tomšič / Dr. Matija Tomšič, Full Professor

Jeziki / Languages: slovenski / Slovenian

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.

Fluorimetrija
Molekularne osnove signala, merjenje in analiza

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 signal analysis, CD - titration usefulness in the study of (induced) asymmetry of the molecules.

Fluorimetry
Molecular basis of the signal, measurement and

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, reološke lastnosti, viskoznost)

Difuzija in dinamika molekul v raztopinah

Koeficient lastne difuzije, koeficient kemijske difuzije. Pomen koeficienta difuzije pri proučevanju transportnih in asociacijskih pojavov v raztopinah. Eksperimentalno določanje koeficientov difuzije. Raziskave dinamike molekul z NMR metodami.

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, rheological properties, viscosity)

Diffusion and dynamics of molecules in solutions

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. Studies of molecular dynamics using NMR methods.

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, Clarendon 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 sistemov, raznih raztopin ter fizikalnih značilnosti kemijskih reakcij oziroma procesov.

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 various physical properties of chemical reactions and processes.

<p><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.</p>	<p><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.</p>
<p><u>Prenosljive spretnosti</u> Sistematičnost pristopa pri reševanju projektne naloge, zbiranje literature, ovrednotenje in poročanje o rezultatih projekta.</p>	<p><u>Skill-transference Ability</u> Systematic approach to solving the experimental problems, collecting of literature, evaluating and reporting on the results of the project.</p>

Metode poučevanja in učenja:

Predavanja, eksperimentalne praktične vaje, projektna vaja.

Learning and Teaching Methods:

Lectures, seminars, laboratory exercises.

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

Reference nosilca / Lecturer's references:

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

LAH, Jurij, MAIER, Norbert M., LINDNER, Wolfgang, VESNAVER, Gorazd. Thermodynamics of binding of (R)- and (S)-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 fullerenehexamalonate Th-C66(COOH)12 and its alkali and calcium salts. J. Phys. Chem. B, 2008, 112, str. 892-895.

CERAR, Janez, URBIČ, Tomaž: Viscosity and electrophoretic mobility of cesium fullerenehexamalonate in aqueous solutions : comparing experiments and theories on nanometer-sized spherical polyelectrolyte. J. Phys. Chem. B, 2008, 112, str. 12240-12248.

ŠKERJANC, Jože, KOGEJ, Ksenija, CERAR, Janez: Equilibrium and transport properties of alkylpyridinium bromides. Langmuir, 1999, 15, str. 5023-5028.

TOMŠIČ, Matija, BEŠTER-ROGAČ, Marija, JAMNIK, Andrej, KUNZ, Werner, TOURAUD, Didier, BERGMANN, Alexander, GLATTER, Otto. Nonionic surfactant Brij 35 in water and in various simple

alcohols : structural investigations by small-angle x-ray scattering and dynamic light scattering. J. phys. chem., B Condens. mater. surf. interfaces biophys., 2004, vol. 108, no. 22, str. 7021-7032

TOMŠIČ, Matija, JAMNIK, Andrej, FRITZ, Gerhard, GLATTER, Otto, VLČEK, Lukáš. Structural properties of pure simple alcohols from ethanol, propanol, butanol, pentanol, to hexanol : comparing Monte Carlo simulations with experimental SAXS data. J. phys. chem., B Condens. mater. surf. interfaces biophys., 2007, vol. 111, no. 7, str. 1738-1751.

TOMŠIČ, Matija, GLATTER, Otto. From bulk to dispersed hierarchically organized lipid phase systems. V: IGLIČ, Aleš (ur.). Advances in planar lipid bilayers and liposomes : volume 12, (Advances in planar lipid bilayers and liposomes). Amsterdam; Elsevier: Academic Press, cop. 2010, str. 167-200.

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