UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	KEMIJSKA TERMODINAMIKA
Course Title:	CHEMICAL THERMODYNAMICS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
UŠP Kemijsko inženirstvo, 1. stopnja	**/**	**2.**	**3.**
USP Chemical Egineering, 1st Cycle	**/**	**2nd**	**3rd**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: IN114

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
60	**15**	**/**	**/**	**/**	**75**	**5**

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

Jeziki / Languages:

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

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

Vsebina:	Content (Syllabus outline):
Osnovni pojmi Sistem, lastnosti sistema, stanje sistema, funkcije stanja in funkcije poti, ravnotežje. Enačbe stanja: Plinski zakoni, enačba stanja idealnega plina, van der Waalsova enačba, virialna enačba, enačba stanja za plinske zmesi. Kritični pojavi. **Zakoni termodinamike** *I. zakon termodinamike:* Energija, toplota, delo. Reverzibilni in ireverzibilni procesi. Entalpija. Termokemija in termokemijske enačbe. *II. zakon termodinamike:* Toplotni stroji: izkoristek, Carnotov krožni proces. Entropija.	**Basic concepts** System and its properties, system state, state functions and path functions, equilibrium. Equations of state: Gas laws, equation of state for ideal gas, van der Waals equation, virial equation, equation of state for gas mixtures. Critical phenomena. **Laws of thermodynamics** I. Law of thermodynamics: energy, heat, work. Reversible and irreversible processes. Enthalpy. Thermochemistry and thermochemical equations. II. Law of Thermodynamics: Heat engines: efficiency, Carnot cycle. Entropy. Changes in

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Spremembe entropije pri reverzibilnih in ireverzibilnih procesih. Ravnotežni pogoji za zaprte sisteme: prosta energija, termodinamski potenciali, odvisnost termodinamskih funkcij od tlaka in temperature. III. zakon termodinamike.	entropy in reversible and irreversible processes. Equilibrium conditions for closed systems: free energy, thermodynamic potentials, the dependence of thermodynamic functions on pressure and temperature. III. Law of thermodynamics.
Odprti sistemi Faze, komponente, prostostne stopnje. Fazno pravilo. Clapeyronova in Clausius-Clapeyronova enačba. Fazni diagrami.	**Open systems** Phase, components, degrees of freedom. Phase rule. Clapeyron and Clausius-Clapeyron equation. Phase diagrams.
Raztopine Idealne in neidealne raztopine, Raoultov zakon, Henryjev zakon. Parcialne molske količine, kemijski potencial. Fugativnost, aktivnost in koeficient aktivnosti. Standardna stanja. Termodinamika mešanja. Koligativne lastnosti: Osmozni tlak, znižanje zmrzišča, zvišanje vrelišča.	**Solutions** Ideal and non-ideal solutions, Raoult's law , Henry's law. Partial molar quantities, chemical potential. Fugacity, activity and activity coefficient. Standard states. Thermodynamics of mixing. Colligative properties: osmotic pressure, lowering the freezing point, boiling point increase.
Kemijsko ravnotežje Konstanta ravnotežja. Homogeno ravnotežje v plinasti in tekoči fazi. Heterogena ravnotežja. Le Chatelierov princip.	**Chemical equilibrium** Equilibrium constant. Homogeneous equilibrium in gaseous and liquid phase. Heterogeneous equilibria. Le Chatelier principle

Temeljna literatura in viri / Readings:

- A. Jamnik, Fizikalna kemija (1. izdaja), založba FKKT (2013) (80%), ISBN: 978-961-6756-39-6 (1. zvezek) (20%), ISBN: 978-961-6756-40-2 (2. zvezek).
- Physical Chemistry, P. Atkins in J. de Paula, Oxford University Press, 8. Izdaja (2006), 1050 str., (30%), ISBN 9780198700722.
- Physical Chemistry, W. Moore, Prentice-Hall, New Jersey, 5. Izdaja (1972), str. 1-570, (50%), ISBN 0582442346.

Cilji in kompetence:	**Objectives and Competences:**
Cilj predmeta je spoznavanje povezave med fizikalnimi in kemijskimi pojavi ter med fizikalnimi in kemijskimi lastnostmi snovi. Študent se seznani s temeljnimi fizikalno kemijskimi količinami, s katerimi popisujemo stanje sistemov, ter s povezavo med njimi. Spozna splošne zakonitosti pri opisu različnih problemov iz naravoslovja in fizikalno-matematične metode za njihovo reševanje. Študenti si pri predmetu pridobijo naslednje specifične kompetence:	The objective of this subject is to study the relation between physical and chemical phenomena and between physical and chemical properties of the matter. Students get acquainted with the fundamental physico-chemical quantities with which we describe the state of the systems, and the relation between them. Students learn about general laws useful in describing various problems in science and get acquainted with physico-mathematical methods to solve them.

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- razumevanje termodinamskih zakonov in termodinamskih funkcij stanja ter njihova uporaba pri kemijskih reakcijah in fizikalnih procesih - uporaba kriterijev za napoved spontanosti poljubnih procesov pri različnih konstantnih pogojih - uporaba različnih načinov, s katerimi vplivamo na kemijsko ravnotežje - sistematičnost pristopa pri reševanju teorijskih problemov in računskih nalog	Students of the course gain the following specific competencies: - Understanding the thermodynamic laws and thermodynamic state functions and their use in chemical reactions and physical processes - Use of criteria for predicting the spontaneity of processes at different constant conditions - Use various ways for influencing the chemical equilibrium. - A systematic approach in solving theoretical and numerical problems.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Poznavanje osnovnih fizikalno-kemijskih količin kot so notranja energija, entalpija, prosta energija in entropija. Poznavanje osnovnih zakonov termodinamike. Razumevanje pojmov obrnljivosti (reverzibilnosti) in neobrnljivosti (ireverzibilnosti) procesov. Poznavanje kriterijev za spontanost poteka kemijskih reakcij ter za kemijsko ravnotežje. Razumevanje razlike med termodinamiko (spontanostjo poteka) ter kinetiko (hitrostjo poteka) kemijske reakcije.	<u>Knowledge and Comprehension</u> Knowledge of basic physico-chemical quantities such as internal energy, enthalpy, free energy and entropy. Knowledge of the basic laws of thermodynamics. Understanding the concepts of reversible and irreversible processes. Knowing the criteria for spontaneous chemical reactions and chemical equilibrium. Understanding the difference between thermodynamics (spontaneity) and kinetics (rate) of a chemical reaction.
<u>Uporaba</u> Uporaba tabeliranih fizikalno-kemijskih podatkov (standardne tvorbene entalpije, standardne entropije, toplote faznih prehodov, toplotne kapacitete) pri določanju termodinamike kemijskih reakcij pri različnih pogojih.	<u>Application</u> Using tabulated physico-chemical data (standard enthalpy of formation, standard entropy, heat of phase transitions, heat capacity) in determining the thermodynamics of chemical reactions under different conditions.
<u>Refleksija</u> Pridobitev občutka za fizikalno-matematični način razmišljanja ter spoznanja o splošnih fizikalno-matematičnih metodah za reševanje različnih praktičnih problemov iz naravoslovja. Globlje razumevanje pomena abstraktnih fizikalno-kemijskih pojmov in količin. Kritična presoja pri izbiri kemijske reakcije za pridobivanje določenega produkta.	<u>Analysis</u> The students acquire the feeling for physico-mathematical way of thinking and for cognition about general physico-mathematical methods for the solution of various problems in natural science. Deeper understanding of the significance of abstract physico-chemical principles and properties. A critical assessment of the choice of chemical reactions for the production of a specific product.

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Prenosljive spretnosti Uporaba splošnih naravoslovnih zakonitosti pri študiju inženirskih vsebin, ki so zajete pri drugih predmetih. Uporaba domače in tuje literature.	Skill-transference Ability The use of general natural laws in studying chemical engineering, which are included in other subjects. The use of domestic and foreign literature.

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

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

Reference nosilca / Lecturer's references:

- LAH, Jurij, POHAR, Ciril, VESNAVER, Gorazd. Calorimetric study of the micellization of alkylpyridinium and alkyltrimethylammonium bromides in water. *J. Phys. Chem., B* 2000, 104, 2522-2526.
- LAH, Jurij, MAIER, Norbert M., LINDNER, Wolfgang, VESNAVER, Gorazd. Thermodynamics of binding of (R)- and (S)-dinitrobnzoyl leucine to cinchona alkaloids and their tert-butylcarbamate derivatives in methanol : evaluation of enantioselectivity by spectroscopic (CD, UV) and microcalorimetric (ITC) titrations. *J. Phys. Chem., B* 2001, 105, 1670-1687.
- DROBNAK, Igor, VESNAVER, Gorazd, LAH, Jurij. Model-based thermodynamic analysis of reversible unfolding processes. *J. Phys. Chem., B* 2010, 114, 8713-8722.

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