RĪGAS TEHNISKĀ UNIVERSITĀTE

RTU Course "Physical Chemistry, Thermodynamics"

32000 Faculty of Natural Sciences and Technology

General data

Code	ĶVĶ739
Course title	Physical Chemistry, Thermodynamics
Course status in the programme	Compulsory/Courses of Limited Choice
Responsible instructor	Elīna Sīle
Volume of the course: parts and credits points	1 part, 9.0 credits
Language of instruction	LV, EN
Annotation	The study course provides a comprehension of the thermodynamics of chemical processes. This allows for applying thermodynamic laws to predict the possibility of chemical processes. A student acquires knowledge about the thermodynamic parameters of chemical processes, as well as knowledge about the laws of chemical equilibrium and phase equilibrium. Students will gain knowledge about the methods of calculating the thermodynamic parameters of chemical reactions and the practical application of the calculation results. The study course views the first, second, and third laws of thermodynamics, chemical equilibrium, Clausius-Clapeyron equations, Raoult's law, thermal analysis, physicochemical analysis. The work of studies is focused on the acquisition of theoretical and practical knowledge.
Goals and objectives of the course in terms of competences and skills	The aim of the study course is to provide deep theoretical knowledge about the thermodynamics of chemical processes and the application of their laws in the calculation of practical tasks. The tasks of the study course: 1. To provide skills in calculations of theoretical thermodynamics. 2. To create awareness of how to use the calculations to predict the probability of processes. 3. To develop skills in the calculation of the composition of the chemical system at equilibrium. 4. To develop knowledge about phase and thermal analysis of heterogeneous systems.
Structure and tasks of independent studies	Independent studies of recommended literature, work with reference literature, solving of practical tasks, preparation for tests. Preparation for laboratory work, using theoretical knowledge acquired in lectures and independently. Processing and formatting the results of laboratory works. Completion of homework.
Recommended literature	Obligātā/Obligatory: 1.Alksnis, U., Kļaviņš, Z., Kūka, P., Ruplis, A. Fizikālā un koloidālā ķīmija. Rīga: Zvaigzne, 1990, 425 lpp. 2.Silbey, R. J., Alberty, R. A., Bawendi, M. G. Physical Chemistry. 4th ed. New York: John Wiley and Sons, Inc., 2005, 944 p. 3.Engel, T., Reid, Ph. Physical Chemistry. San Francisco: Pearson Education, Inc., 2006. 1061 p. 4.Atkins, P. W. Physical Chemistry. 3rd ed. New York: W. H. Freeman and Company, 1986. 857 p. 5.Atkins, P., J.de Paula, J. Atkins' Physical Chemistry, Tenth edition, 2014, 1008 p. 6.Laidler, K. J., Meiser, J. H. Physical Chemistry. 3rd ed. Boston – New York: Houghton Mifflin Company, 1999. 1019 p. 7.Obimakinde, J. O., Obimakinde, S. O. Calculations in chemistry. New Delfi, I.K. International Publishing House Pvt.Ltd., 2014. 708p. 8.Balodis, J. Praktiskie darbi fizikālajā ķīmijā. 1 daļa. Rīga: Zvaigzne, 1975, 213 lpp. Papildu/Additional: 1.Zumdahl, S. S., Zumdahl, S. A. Chemistry. Cengage Technology Edition. 9th edition. University of Illinois, Inc.© 2014.1068p.
Course prerequisites	Prerequisites in mathematics, physics, inorganic and organic chemistry.

Course contents

Content	Full- and part-time intramural studies		Part time extramural studies	
	Contact Hours	Indep. work	Contact Hours	Indep. work
The subject and significance of physical chemistry. A brief history of the development of physical chemistry. Classification of physical chemistry. The subject of thermodynamics, fundamental concepts.	1	1	0	0
Energy. The law of conservation of energy. Heat and work. The equivalence of heat and work.	1	0	0	0
Internal energy. The first law of thermodynamics. Balanced processes. Maximum work. The expansion work of an ideal gas in simple processes: isochoric, isobaric, isothermal, and adiabatic processes.	2	1	0	0
Practical work. Entrance examination.	2	4	0	0
Enthalpy. The application of the first law of thermodynamics in the case of ideal gases. Thermochemistry. The heat of chemical reactions.	1	1	0	0
Hess's law. Calorimetry. The heat of formation of chemical compounds. The heat of combustion. The heat of solution.	1	1	0	0
Laboratory work. Calorimetry.	4	4	0	0
Heat capacity. Heat dependence on the temperature. Kirchhoff's law. Spontaneous and nonspontaneous processes.	2	1	0	0

Practical work. The first law of thermodynamics, tasks, and questions.	2	4	0	0
Practical work. Test. The first law of thermodynamics.	2	4	0	0
The second law of thermodynamics. Carnot cycle. Entropy. The methods of entropy calculation.	2	2	0	0
Planck postulate. Absolute values of entropy. The static character of the second law.	2	1	0	0
Applications of the second law. Thermodynamic potentials. Isochoric-isothermal potential. Isobaric-isothermal potential.	1	1	0	0
The equation of maximum work (Gibbs–Helmholtz equation). Nernst heat theorem.	1	1	0	0
Isochoric-isentropic potential. Isobaric-isentropic potential. Characteristic functions. Conditions of equilibrium.	1	1	0	0
Chemical potential. The thermodynamic potentials of real and ideal gasses. Fugacity (volatility).	1	1	0	0
Practical work. The second law of thermodynamics, tasks, and questions.	2	4	0	0
Practical work. Test. The second law of thermodynamics.	2	4	0	0
Chemical equilibrium. Chemical thermodynamics. Characterization of chemical equilibrium. The law of mass action, its thermodynamic expression.	1	1	0	0
The types of expression of an equilibrium constant. Chemical equilibrium in heterogeneous systems.	1	0	0	0
Calculation of the composition of an equilibrium mixture. The influence of pressure and indifferent gas on the value of the equilibrium constant.	1	1	0	0
Shifting equilibrium. Le Chatelier's principle. Isotherm equation of the chemical reaction. Reaction direction. Chemical affinity.	1	0	0	0
Standard Gibbs energy and standard Helmholtz energy of a reaction. The dependence of chemical equilibrium on temperature. Isochors and isobars equations of reaction.	2	1	0	0
The calculation of an equilibrium constant using data from thermodynamic tables. Temkin-Schwarzman’s method. The method of reduced isobaric potential. Combination of chemical equilibria.	2	1	0	0
Laboratory work. Chemical equilibrium of a heterogeneous reaction.	4	4	0	0
Practical work. Chemical equilibrium, tasks, and questions.	2	4	0	0
Phase Equilibria. Phase. Components. Phase rule and its conditions. Application of phase rule.	1	1	0	0
Classification of thermodynamic systems. One-component systems. Phase transition of individual substances. Clausius-Clapeyron equation.	1	0	0	0
Equilibria “liquid-vapor” and “solid – vapor”. The heat of vaporization. The heat of sublimation.	1	1	0	0
Phase diagrams of one-component systems. Water phase diagram. Sulfur phase diagram. Enantiotropy and monotropy.	1	1	0	0
Phase equilibria in binary (two-component) systems. General description of solutions. Intermolecular interactions in solutions. Classification of solutions(ideal, infinite dilution, nonideal solution)	1	1	0	0
Equilibrium “liquid-vapor” in binary systems. Saturated vapor. Raoult's law. Positive and negative deviation from Raoult's law. Dalton’s law.	1	1	0	0
Laboratory work. The mutual solubility of two liquids.	4	4	0	0
Equilibrium diagrams of binary systems. Binary liquid systems with unlimited mutual solubility of components. Vapor pressure diagrams (isotherms) without and with extremes. The lever rule.	1	1	0	0
First Gibbs-Konovalov rule. Second Gibbs'-Konovalov rule. Azeotropic solutions. Binary liquid system’s boiling point diagram (isobar) without and with extremes. Rectification.	1	1	0	0
Laboratory work. The isobars of boiling points (distillation curves).	4	4	0	0
Practical work. Phase equilibria. One-component systems, tasks, and questions.	2	4	0	0
Binary liquid systems with limited solubility. Solubility diagrams if mutual solubility of components increases or reduces with the temperature rise.	1	1	0	0
The phase composition and mass dependence on temperature. Binary liquid system vapor pressure and boiling point diagrams if mutual solubility of components is limited. Steam distillation.	1	1	0	0
Separation of solid solvent from solutions. Cryoscopy. The boiling point of non-volatile substance solutions. Ebullioscopy. Equilibrium between liquid solutions and gases.	1	1	0	0
The solubility of gases in liquids. Henry-Dalton’s law. Gases solubility dependence on temperature. Osmotic pressure. Thermodynamics of osmotic pressure.	1	1	0	0
Laboratory work. Cryoscopy.	4	4	0	0
Laboratory work. Ebullioscopy.	4	4	0	0
Equilibrium “liquid solution – solid body”. Melting diagrams of binary systems. Construction of melting diagrams. Thermal analysis. Melting diagram with a simple eutectic.	2	2	0	0
Schroeder’s equation. Chemical interaction between components of binary systems. Congruent and incongruent melting.	1	1	0	0
Melting diagram of a binary system if component mutually forms a chemical compound that melts congruently.	1	1	0	0
Laboratory work. Thermal analysis.	4	4	0	0
Melting diagram of a binary system if components mutually form a chemical compound that melts incongruently. Solid solutions.	2	2	0	0
Melting diagrams of binary systems if component mutual solubility in liquid and solid physical states is unlimited, and if component mutual solubility in a solid state is limited.	1	1	0	0
Eutectic type melting diagram if component solubility in a solid state is limited. Peritectic type melting diagram if component solubility in solid state is limited.	1	1	0	0
Practical work. Phase equilibria. Binary systems. Equilibrium “liquid-gas”. Equilibrium “solid-liquid”.	2	4	0	0

Physicochemical analysis. The principle of continuity. The principle of conformity. Singular points.	2	2	0	0
A brief characterization of phase diagrams of three-component systems. Techniques for representing the composition of three-component systems. Ternary phase diagram.	2	2	0	0
Laboratory work. Mutual solubility of three liquids.	4	4	0	0
Home test. The first and second law of thermodynamics.	0	8	0	0
Consultation.	20	0	0	0
Exam.	4	9	0	0
Total:	120	120	0	0

Learning outcomes and assessment

Learning outcomes	Assessment methods
Knows the laws of thermodynamics and is able to evaluate thermodynamic processes, their energetic parameters.	The type of assessment: exam, laboratory works, homework, tests. Assessment criteria: a student is able to apply acquired knowledge to analyse thermodynamic parameters of chemical processes.
Is able to use the acquired knowledge and skills in solving tasks.	The type of assessment: exam, laboratory works, homework, tests. Assessment criteria: a student is able to perform thermodynamic calculations.
Is able to use knowledge and results of theoretical calculations to assess the feasibility of a chemical process and to obtain a final result.	The type of assessment: exam, laboratory works, tests. Assessment criteria: a student is able to apply acquired knowledge and the results of thermodynamic calculation of energetic parameters to assess the feasibility of the chemical process.
Is able to perform phase and thermal analysis of heterogeneous systems.	The type of assessment: exam, laboratory works, tests. Assessment criteria: a student is able to solve tasks about heterogeneous equilibrium, he is able to perform thermal analysis of systems experimentally.
Is able to critically compare experimental results with data published in the literature.	The type of assessment: the preparation of the reports of laboratory works, their formation, and defence. Assessment criteria: a student is able to apply acquired knowledge and results of calculation to analyse research.

Evaluation criteria of study results

Criterion	%
Exam	50
Tests	20
Laboratory works	15
Homework	15
Total:	100

Study subject structure

Part	CP	Hours			Tests		
		Lectures	Practical	Lab.	Test	Exam	Work
1.	9.0	3.0	1.0	2.0		*	