AL-FARABI KAZAKH NATIONAL UNIVERSITY

Faculty of chemistry and chemical technology
Department of physical chemistry, catalysis and petrochemistry

Program of the final exam on discipline

60317 Theory and Problems of Physical Chemistry

Educational program:
«7M05301-Chemistry»

Almaty 2023

The program of the final exam is composed by the lecturer of the Department of Physical Chemistry, Catalysis and Petrochemistry, PhD Supiyeva Zh.A.

Reviewed and recommended at the meeting of the department of physical chemistry, catalysis and petrochemistry

«6» October 2023, Protocol №4

Head of department _____ Ye.A.Aubakirov

Introduction

Exam form - standard, written.
Exam platform: UC Univer
Exam type - offline
Control of the exam - video cameras in the classroom and the teacher.
Exam duration: 3 hours.

Topics on which exam papers will be compiled

1. Concepts of physical and chemical (hydrate) theory of solutions.
2. Energy of the crystal lattice. The Born, Kapustinsky model and the Born-Haber cycle for calculating the energy of a crystal lattice.
3. Solvation energy. Born model and Born-Haber cycle for calculating solvation energy. Ionophores and ionogens.
4. Modern concepts about the mechanism of formation of solutions of strong and weak electrolytes. Chemical and real energy of solvation.
5. The modern concept of thermodynamics of ionic solvation in solutions, determination of enthalpy, Gibbs energy and entropy of formation of ions in solution.
6. Intermolecular interaction in solutions of strong electrolytes. Lewis thermodynamic theory, activity, activity coefficient.
7. Debye and Hückel's ideas about the nature of the average ion activity coefficient. Modern concept of the theory of strong electrolytes.
8. The influence of the ionic strength of a solution on the rate of ionic reactions. Application of the Debye-Hückel theory to solutions of weak electrolytes.
9. Fundamentals of statistical thermodynamics. Boltzmann's law on the distribution of particles in macrosystems.
10. Gibbs statistical ensembles. Total particle energy. Energy distribution of molecules, Boltzmann's law.
11. Statistical sum on the state of the system and molecule. Relationship between the molecular sum by state and thermodynamic functions.
12. Theoretical foundations of the theory of active collisions. Methods for determining rate, rate constants for various types of reactions.
13. Theoretical foundations of the theory of the activated complex, the Eyring model, the basic equation of the theory of the transition state. Potential energy surface.
14. Statistical and thermodynamic aspects of the transition state theory. Methods for determining the rate, rate constants of complex reactions.
15. Comparative analysis of active collision theories and transition state theory. Distinctive features and applications of these theories for the kinetic analysis of complex reaction reactions.

Exam rules

1. The student needs to come to the classroom 15 minutes before the start of the exam and prepare, sign on the attendance sheet and sit in the seat indicated on the attendance sheet. Bring your ID, pen and pencil.

2. In the event that a substitute person appears at the written examination, the teacher on duty draws up a corresponding act of violation of this document.

3. Student being late for the exam is not allowed.

Prohibited during the exam:

1. Carry and/or use cheat sheets, cell phones, smart watches, other technical and other means that can be used for unauthorized access to auxiliary information.

2. Talk with other students and strangers.

3. Record your full name and/or other identifying information in your responses.

Instructions for students

1. If a student violates one or more of these points, a certificate of cancellation of the examination work is filled out and given (unsatisfactory) for the discipline.

2. If a student appears for the exam and refuses to answer the ticket, passing the exam is graded “F”.

3. In the absence of a valid reason, failure to appear for the exam is assessed as an “F” grade.

4. For repeated violation of these Rules during the exam, the student is presented for consideration by the Faculty Council on Ethics.

5. The final grade for the discipline can be canceled within 1 month after the exam if students are found to have violated the Instructions for conducting final control using distance learning technologies and/or rules of conduct during the exam: using cheat sheets, cell phones, negotiating, etc. d. based on recordings from surveillance cameras with filling out the Report. The act is not subject to cancellation, appeal or appeal.

6. All violations during the exam are recorded in the student’s transcript.

Grading Policy

The ticket will contain 3 tasks (questions). Each task is worth 100 points. The final result will be the sum of all questions on the ticket divided by the number of criteria.

RUBRICTOR FOR CRITERIAL ASSESSMENT OF FINAL CONTROL

Criterion/ score	Descriptors				
	Criterion/score	**Fine**	**Satisfactorily**	**Unsatisfactory**	
	90–100% (27-30 баллов)	**70–89% (21-26 баллов)**	**50–69% (15-20 баллов)**	**25–49% (8-14 баллов)**	**0–24% (0-7 баллов)**
Knowledge and understanding of course theory and concepts	A complete, detailed answer to the question posed is given, the totality of conscious knowledge about an object is shown, manifested in the free operation of concepts, the ability to identify its essential and non-essential features, and cause-and-effect relationships. Knowledge about an object is demonstrated against the background of understanding it in the system of a given science and interdisciplinary connections.	A complete, detailed answer to the question posed is given, the main provisions of the topic are conclusively revealed; the answer shows a clear structure that reflects the essence of the concepts, theories, and phenomena being revealed.	An insufficiently complete and consistent answer to the question posed is given, but at the same time the ability to identify essential and non-essential features and cause-and-effect relationships is demonstrated. There may be 1-2 mistakes made in defining basic concepts, which the student finds difficult to correct on his own.	An incomplete answer was given, gross errors were made in determining the essence of the concepts, theories, and phenomena being revealed, due to the student's lack of understanding of their essential and non-essential features and connections. The answer contains no conclusions.	An incomplete answer was given, representing scattered knowledge on the topic of the question with significant errors in definitions.

Compliance with scientific, logical and consistent presentation	The answer is formulated in scientific terms, presented in literary language, logical, consistent, demonstrative, and demonstrates the student's author's position.	The answer is stated in literary language in scientific terms. There were some shortcomings in the answer, which were corrected by the student using teacher.	The answer is logical and stated in scientific terms. There may be 1-2 mistakes made in defining basic concepts, which the student finds difficult to correct on his own.	The logic and consistency of presentation have significant violations. Additional and clarifying questions from the teacher do not lead to correction of the student's answer not only to the question posed, but also to other questions in the discipline.	There is fragmentation and illogical presentation. The student does not realize the connection of this concept, theory of phenomenon with other objects of the discipline. There are no conclusions specification and evidence of presentation. Speech is illiterate.
Application of the selected methodology and technology to specific practical tasks	Complete completion of the educational assignment, a detailed, reasoned answer to the question posed, followed by solving practical problems of the course; generalizes his practical skills.	Partial completion of the educational assignment, incomplete, sometimes reasoned answer to the question posed with an incomplete solution to the practical problems of the course; illiterate use of scientific language norms in the course; partially generalizes his practical skills.	The material is presented in fragments, in violation of logical sequence, factual and semantic inaccuracies are made, and theoretical knowledge of the course is used superficially.	An irrational method of solving a task or an insufficiently thought-out answer plan; inability to solve problems, perform tasks in general; making mistakes and omissions that exceeds the norm.	Inability to apply knowledge and algorithms to solve tasks; inability to draw conclusions and generalizations. Violation of the Rules for final control.

Example of calculating the final score

№	Point / Criterion	«Excellent»	«Good»	«Satisfactorily»	«Unsatisfactory»	
		90-100 %	**70-89 %**	**50-69 %**	**25-49 %**	**0-24 %**
	Criterion 1	100				
	Criterion 2		75			
	Criterion 3		75			
	Final %	**100**	**150**			100+ 75+75 = 250 **250 / 3 criterion = 83,3** **Final score in % = 83**

Recommended literature sources for exam preparation

Main:

1. C.R. Metz Theory and Problems of Physical Chemistry / McGraw-Hill, 1974.
2. Clyde R. Metz Theory and Problems of Physical Chemistry / McGraw-Hill; First edition (January 1, 1976).
3. Dr. RK Gupta Problems in Physical Chemistry / JEE Main and Advanced - 518 p.
4. Kenneth Schmitz Physical Chemistry Concepts and Theory /1st Edition - November 11, 2016.
5. Оспанова А.К., Шабикова Г.Х., Сыздыкова Л.И. Физикалық химияның теориялары мен мәселері. Алматы. 2021. с 191.
6. Г.Х. Шабикова, Л.И. Сыздыкова Современное состояние теории сольватации и растворения. Алматы.2010.

Additional:

1.Geerlings, P.; De Proft, F. Chemical Reactivity as Described by Quantum Chemical Methods. Int. J. Mol. Sci. 2002, 3, 276-309. https://doi.org/10.3390/i3040276

Internet resources:

1. http://elibrary.kaznu.kz/ru
2.http://sciencedirect.com/