

**AL-FARABI KAZAKH NATIONAL UNIVERSITY**  
**Faculty of Chemistry and Chemical Technology**  
**Department of Physical Chemistry, Catalysis and Petrochemistry**

**Final exam program for the discipline**

**PMS 5304 «Applied molecular spectroscopy»**

**Educational program:**

**7M05301 - Chemistry**

**Almaty 2022**

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

Reviewed and recommended at the meeting of the Department of Physical Chemistry, Catalysis and Petrochemistry  
at “10” February 2022, protocol No 8

Head of the department \_\_\_\_\_ Ye.A. Aubakirov  
(signature)

## Introduction

**Exam format:** synchronous.

**Exam form:** Oral exam.

**Exam platform:** Zoom.

**Exam type:** online.

**Exam control:** video recording.

**The exam lasts:** Preparation time is 5 minutes; the response time is 20 minutes.

**On the exam in this discipline** the ticket will have 2 tasks (questions).

### Topics for which test tasks will be drawn up

1. Introduction to the theory of molecular spectra. Molecular spectroscopy, general principles, classification and application. Units of measurement and designations adopted in spectroscopy. Characteristics of electromagnetic radiation. Classification of types of spectroscopy by regions of the electromagnetic spectrum.

2. Energy states of the molecule. Separation of energy into electronic, vibrational and rotational components. Dependence of the potential energy of a molecule on the internuclear distance. Possible types of transitions of molecules from one energy state to another. Interaction of radiation with matter. Spectral lines. Formation of spectra of molecules.

3. Statistical distribution of molecules by energy states. Relative population of energy states of molecules. Calculation of thermodynamic functions via sums over states.

4. Registration of the absorption spectrum. Selection rules. Transition probabilities. Spectral line intensity. Electric dipole moment. The laws of light absorption and the intensity of the bands in the spectra. Absorption band width.

5. Rotation and rotational spectra of molecules. Theory of rotational spectra. Conditions for observing rotational spectra. Rotation and rotational spectra of diatomic molecules. Rotation of polyatomic molecules. Structural information obtained from the rotational spectra of molecules.

6. Vibrational spectroscopy. Characteristics of IR radiation. Vibrations of diatomic molecules AB. Harmonic oscillator (vibrational energy, frequency, selection rule). Anharmonic oscillator.

7. Vibrations of polyatomic molecules. Types of vibrations. Selection rules. Group fluctuations. Characteristic frequencies of IR absorption of the main classes of compounds. Structural molecular analysis by infrared absorption spectrum.

8. Raman Spectroscopy (RS). Theoretical basis. Rayleigh equation. Raman scattering. Selection rules. Areas of use.

9. Electronic spectroscopy. Electromagnetic spectrum. Franck-Condon principle. Origin of absorption bands. Intensity of absorption bands. Characteristics of oscillation frequencies and electronic transitions. Electronic spectroscopy of transition metal complexes and charge transfer complexes.

10. Electronic spectroscopy. Spectrophotometric analysis of colored compounds. Types of photometric systems. Elimination of the influence of related components. Choice of optimal conditions for carrying out the spectrophotometric reaction. Sensitivity of photometric methods.

11. Electronic spectroscopy. Methods of quantitative absorption-spectroscopic analysis. Methods for the determination of one substance. Analysis of multicomponent systems. Spectrophotometric titration method with and without indicator. Processing the results of spectrophotometric measurements.

12. Electronic spectroscopy. Application of the method of absorption spectroscopy to study equilibria in solutions. Calculation of dissociation constants of organic reagents. Determination of the composition and stability constants of complex compounds.

13. Luminescent method. Basic principles. Spectra of luminescence. Qualitative luminescent analysis. Equipment for luminescent analysis.

14. Boiling point (vapor pressure) - composition (t, P - x) diagrams. Gibbs-Konovalov laws I and II.

15. Ebulliometry. Cryometry. Determination of the molecular weight and molecular state of the solute from cryometric or ebulliometric data. Isotonic Van't Hoff coefficient.

### **Rules for conducting the exam**

#### **Oral exam: traditional - answers to questions**

**Important!** The exam is held according to a schedule that should be known in advance to students and teachers.

The organizer of the exam-conference-the teacher or a member of the exam committee who will take the exam, plans the conference in advance on the selected platform and sends an invitation to the exam participants.

On the day of the exam, for 30 minutes, the teacher reminds students about the beginning of the exam in the general chat. If necessary, change the communication platform.

If zoom is used, the examiner should divide the exam into periods of 30-40 minutes for reconnection.

The student must complete the exam in one session.

It is forbidden to start responding in the same session and end after reconnecting.

If the response is interrupted during a new connection, the examiner issues a new ticket to the examinee.

**Important!** The video recording is turned off only at the end of the exam, when the answers of all the examinees are accepted.

#### **General procedure**

After connecting all the participants online in the conference, the teacher or member of the commission:

- starts **Video recording** of the exam;
- greets the participants of the exam;
- warns that video is being recorded;
- announces the rules of the exam;
- names the order of the examinees;
- names the preparation time (at the discretion of the teacher);
- names the response time (at the discretion of the teacher);
- gives permission to compose answers, if necessary, on paper with a pen;
- requires the examinee to show his answer sheet before starting the answer;
- allows other examinees to be on standby - not to be in front of the camera all the time, but not to leave the meeting;
- gives the surname, name and patronymic of the examinee;
- asks the examinee to show the room in which he is located on a video camera - there should be no strangers in the room, no additional sources of information (if possible from the student's side);
- warns about the ban on the use of additional sources of information;
- say to a student: "You can open your ticket";
- gives time for preparation - at the discretion of the teacher and the commission;
- controls the preparation process via video link, making comments if necessary;
- accepts the answer from the examinee;
- allows the examiner to leave the meeting.

The same procedure is repeated with each exam participant.

#### **Student instruction**

**The student must:**

1. Have a computer or laptop with a webcam and access to the Internet.
2. Timely before the start of the exam, connect the computer and the video camera and do not turn off the video camera during the exam.
3. Before the start of the exam, it is mandatory to pass identity verification by showing an identification document on a webcam (identity card).

**Important! You must have with you: identity card.** In the absence of supporting documents, the student is not allowed to take the exam! If a third party replaces a student, both the student and the third party are brought to disciplinary responsibility.

4. Carefully read and follow the instructions for passing the exam.
5. The answer to each examination question should be stated consistently, clearly.
6. If the student for technical reasons could not connect, then it is necessary to report the technical problem to the adviser within three hours after the start of the exam.
7. The student has the right to submit an appeal within 24 hours from the moment the grade for the exam in the “Univer” system is set in the event that: the exam ticket contains an incorrect question or a question that does not correspond to the curriculum of the discipline.

**Attention!** The use of headphones, including wireless headphones, is permitted only at the time of receiving additional questions from members of the examination committee. In all other cases, the use of headphones is FORBIDDEN!

**It is prohibited:**

1. To have with you during the exam unauthorized aids (cribs, cell phones (on or off), smart watches, other electronic devices, etc.).
2. To make noise, talk, get up and leave the webcam field, premises.
3. To seek help and provide access to the computer to third parties during the exam.
4. To look away from the computer screen.
5. Additionally, to open the tabs of browsers, instant messengers, MO Excel, additional monitors and computer equipment, except for the one that is directly used for the exam.
6. To use books, drafts, calculators without permission.
7. To turn off or reduce the level of sensitivity of the microphone to sound during the exam.

**Important!**

1. A student who has committed a violation of any of the above requirements, which was recorded by the act, will be given an “F” (“unsatisfactory”) mark for the discipline.
2. The opening of unauthorized educational and methodological materials, electronic means of communication in the student during the exam, as well as violation of these Regulations, is the basis for making a decision to cancel the assessment results and give the grade “unsatisfactory”, regardless of whether they were used in the exam or not.

**Important!**

1. Questions are automatically generated by the Deputy Dean. The student is prohibited from opening the exam ticket until the teacher-examiner says “You can open your ticket”.
2. After opening a ticket in the university system, the time countdown begins.
3. The ticket will have 2 tasks (questions).
4. Read the exam rules carefully and follow them. Answer the teacher’s questions and follow all his instructions.

**Evaluation policy**

The ticket will have 2 tasks (questions). The tasks are estimated in sum as 100 points. The 1st task – 50, the second task – 50. The total result will be the sum for all questions of the ticket.

### **Recommended literature sources for exam preparation**

1. Fundamentals of Molecular Spectroscopy [Banwell, Colin N.] on Amazon.com. ... Publisher: McGraw-Hill Book Co Ltd; 3rd edition (May 1, 1983).
2. Chang R. Basic Principles of Spectroscopy, Krieger, 1978.
3. Молекулярная спектроскопия: основы теории и практика: Учебное пособие / Под ред. проф. Ф.Ф. Литвина. - М.: НИЦ Инфра-М, 2013. –263 с.
4. Пентин Ю.А., Курамшина Г.М. Основы молекулярной спектроскопии. – Лаборатория знаний Бином, 2013. – 398 с.
5. Ельяшевич М.А. Атомная и молекулярная спектроскопия: Общие вопросы спектроскопии. - Книжный дом "ЛИБРОКОМ", 2014. – 240 с.
6. Молекулярная спектроскопия: основы теории и практика: Учебное пособие / Под ред. проф. Ф.Ф. Литвина. - М.: НИЦ Инфра-М, 2013. - 263 с.
7. Фриш С.Э. Оптические спектры молекул: Учебное пособие. - СПб.: Издательство "Лань", 2010. - 656 с. // <http://e.lanbook.com/view/book/625/>