Federal State Autonomous Educational Institution for Higher Education
Peoples' Friendship University of Russia named after P. Lumumba
(RUDN University)

Science faculty

educational division (faculty/institute/academy) as higher education programme developer

COURSE SYLLABUS

MOLECULAR SPECTRAL ANALYSIS

course title

Recommended by the Didactic Council for the Education Field of:

04.04.01 Chemistry

field of studies / speciality code and title

The course instruction is implemented within the professional education programme of higher education:

«Fundamental and applied chemistry»

higher education programme profile/specialisation title

2024

1. COURSE GOAL(s)

The goal of the course of «Molecular spectral analysis » is to obtain a general understanding of the basics of infrared spectroscopy, the skills to obtain and analyze of organic compounds' spectral data.

2. REQUIREMENTS FOR LEARNING OUTCOMES

Mastering the discipline "Molecular spectral analysis" expects students to acquire the following competences /competences in part.

Table 2.1. List of competences that students acquire through the course stud

Competence code	**Competence descriptor**	**Competence formation indicators** (within this course)
PC-1	To be able to plan work and choose adequate methods for solving research problems in the chosen field of chemistry, chemical technology or sciences related to chemistry	PC-1.1. To draw up a general plan of research and detailed plans for individual stages.
		PC-1.2. To select experimental and computational-theoretical methods for solving the problem based on the available material and time resources.
PC-2	To be able to base on a critical analysis of the results of research and development, to assess the prospects for their practical application and the continuation of work in the chosen field of chemistry, chemical technology or sciences related to chemistry	PC-2.2. To determine possible directions for the development of work and prospects for the practical application of the results obtained

3. COURSE IN HIGHER EDUCATION PROGRAMME STRUCTURE

The course refers to the elective component of (B1) block of the higher educational programme curriculum.

Within the higher education programme students also master other (modules) and / or internships that contribute to the achievement of the expected learning outcomes as results of the course study.

Table 3.1. The list of the higher education programme components/disciplines that contribute to the achievement of the expected learning outcomes as the course study results

Competence code	**Competence descriptor**	**Previous courses/modules***	**Subsequent courses/modules***
M-PC-1-s	To be able to plan work and choose adequate methods for solving research problems in the chosen field of chemistry, chemical	Methods of organic chemistry Theoretical organic chemistry The method of working with databases	Chemistry of natural compounds Chemistry of heterocyclic compounds Mass spectrometry of organic compounds

Competence code	Competence descriptor	Previous courses/modules*	Subsequent courses/modules*
	technology or sciences related to chemistry	Fundamentals of biotechnology Research work Experimental research methods in the chemistry	Stereochemistry Fundamentals of drug design Research work Undergraduate practice
PC-2	To be able to base on a critical analysis of the results of research and development, to assess the prospects for their practical application and the continuation of work in the chosen field of chemistry, chemical technology or sciences related to chemistry	Experimental research methods in the chemistry	Mass spectrometry of organic compounds Research work Undergraduate practice

* To be filled in according to the competence matrix of the higher education programme.

4. COURSE WORKLOAD AND ACADEMIC ACTIVITIES

The total workload of the course is 3 credits.

Table 4.1 Types of academic activities during the periods of higher education programme mastering (full-time training)

Types of academic activities		Total academic hours	Semesters			
			1	2	3	4
Contact academic hours		*54*		*54*		
including:						
Lectures (**LC**)		36		36		
Lab Works (**LW**)		18		18		
Seminars (workshops/tutorials) (S)						
Self-studies		*36*		*36*		
Evaluation and assessment (exam/passing/failing grade)		*18*		*18*		
Course workload	academic hours_	**108**		**108**		
	credits	**3**		**3**		

5. COURSE CONTENTS

Table 5.1. Course contents and academic activities types

Course module title	Course module contents (topics)	Academic activities types
Section 1. Basics of Molecular spectral analysis	Topic 1.1. Electromagnetic spectrum. Basic characteristics of radiation. Interaction of radiation with matter. Main features of atomic and molecular spectra.	LC
	Topic 1.2. Classification of methods of molecular	LC

Course module title	Course module contents (topics)	Academic activities types
	spectral analysis. Significance of molecular spectral analysis in chemistry.	
Section 2. Basics of IR spectroscopy	Topic 2.1 Structural features of polyatomic molecules. Hooke's law and the Schrödinger equation as applied to polyatomic molecules. The main tasks of the theory of vibrations of molecules. Vibrations of a polyatomic molecule as an interconnected system. The number of possible oscillations. Normal oscillations and their properties. Classification of normal vibrations.	LC
	Topic 2.2. Symmetry of molecules. Elements of the classical theory of infrared absorption spectra. Fundamentals of the classical theory of Raman scattering. Selection rules. Frequency characteristic in the vibrational spectrum of a molecule. Peculiarities of Quantum-Chemical Consideration of Vibrations of Polyatomic Molecules.	LC, LW
Section 3. Basics of quantitative IR spectroscopy.	Topic 3.1. The law of absorption of light. Methods for representing spectrophotometric quantities. Instrumental and physico-chemical causes of deviation from the Bouguer-Lambert-Beer law. Factors determining the integrated intensity of absorption bands in infrared spectra. Extrapolation method of Burgen and others. Method of direct integration. correction method.	LC
	Topic 3.2. On the accuracy of measuring the intensities of infrared absorption bands. Absolute intensities in the infrared spectra of molecules	LC, LW
Section 4. Practical aspects of registering of IR spectra	Topic 4.1. General characteristics of IR spectrometers. Sources of radiation. Monochromators. Infrared receivers. Amplifying and recording devices. Modern models of infrared spectrometers. Calibration of prism spectrometers.	LC, LW
	Topic 4.2. Sample preparation technique for analysis.	
Section 5. IR spectroscopy of organic compounds	Topic 5.1. IR spectroscopy of saturated hydrocarbons, olefinic hydrocarbons, acetylenic hydrocarbons, aromatic hydrocarbons, halo-organic compounds, carbonyl- and hydroxyl-containing compounds, amines.	LC, LW
Section 6. Principles of UV spectroscopy	Topic 6.1. The nature of the ESP (electronic absorption spectra). Classification of electronic transitions in a molecule and their assignment. ESP band intensities and selection rules.	LC, LW
	Topic 6.2. The concept of chromophores, auxochromes and conjugated chromophores.	LC, LW

* - to be filled in only for **full** -time training: *LC - lectures; LW - lab work; S - seminars.*

6. CLASSROOM EQUIPMENT AND TECHNOLOGY SUPPORT REQUIREMENTS

Table 6.1. Classroom equipment and technology support requirements

Type of academic activities	**Classroom equipment**	**Specialised educational / laboratory equipment, software, and materials for course study** (if necessary)
Lecture	A lecture hall for lecture-type classes, equipped with a set of specialised furniture; board (screen) and technical means of multimedia presentations.	
Lab work	A classroom for laboratory work, individual consultations, current and mid-term assessment; equipped with a set of specialised furniture and machinery.	Room is equipped with a set of specialized furniture; specialized equipment of the spectroscopy laboratory: manual press, scales, consumables for sample preparation, IR spectrometer
Self-studies	A classroom for independent work of students (can be used for seminars and consultations), equipped with a set of specialised furniture and computers with access to the electronic information and educational environment.	

* The premises for students' self-studies are subject to **MANDATORY** mention

7. RESOURCES RECOMMENDED FOR COURSE STUDY

Main readings:

1. Sindhu, P. S. Fundamentals of Molecular spectral analysis . New Age International, 2006.
2. Hollas, John Michael. Basic atomic and Molecular spectral analysis . Vol. 11. Royal Society of Chemistry, 2002.
3. Rao, K. Narahari, ed. Molecular spectral analysis : modern research. Elsevier, 2012.

Additional readings:

4. McHale, Jeanne L. Molecular spectral analysis . CRC Press, 2017.
5. Mirabella, Francis M., ed. Modern techniques in applied Molecular spectral analysis . Vol. 14. John Wiley & Sons, 1998.

Internet sources

1. Electronic libraries (EL) of RUDN University and other institutions, to which university students have access on the basis of concluded agreements:

- RUDN Electronic Library System (RUDN ELS) http://lib.rudn.ru/MegaPro/Web
- EL "University Library Online" http://www.biblioclub.ru
- EL "Yurayt" http://www.biblio-online.ru
- EL "Student Consultant" www.studentlibrary.ru

- EL "Lan" http://e.lanbook.com/
- EL "Trinity Bridge"

Databases and search engines:

- electronic fund of legal and normative-technical documentation http://docs.cntd.ru/
- Yandex search engine https://www.yandex.ru/
- Google search engine https://www.google.ru/
- abstract database SCOPUS http://www.elsevierscience.ru/products/scopus/

*Training toolkit for self- studies to master the course *:*

1. The set of lectures on the course "Molecular spectral analysis".
2. The laboratory workshop on the course "Molecular spectral analysis".

* The training toolkit for self- studies to master the course is placed on the course page in the university telecommunication training and information system under the set procedure.

8. ASSESSMENT AND EVALUATION TOOLKITS

ASSESSMENT TOOLKIT AND GRADING SYSTEM* FOR EVALUATION OF STUDENTS' COMPETENCES LEVEL UPON COURSE COMPLETION

The assessment toolkit and the grading system* to evaluate the competences formation level (competences in part) upon the course study completion are specified in the Appendix to the course syllabus.

* The assessment toolkit and the grading system are formed on the basis of the requirements of the relevant local normative act of RUDN University (regulations / order).

DEVELOPERS:

Assistant professor, Organic Chemistry Department		**R.S.Borisov**
Position, Department	Signature	name and surname

HEAD OF EDUCATIONAL DEPARTMENT:

Organic Chemistry Department		**L. G. Voskressensky**
Name of Department		name and surname

HEAD
OF HIGHER EDUCATION PROGRAMME:

Dean of Science faculty, Head of the Department of Organic Chemistry		**L. G. Voskressensky**
Position, Department	Signature	name and surname