

TARAS SHEVCHENKO NATIONAL UNIVERSITY OF KYIV

CHEMICAL DEPARTMENT



«APPROVED»

Deputy dean for academic work

Nataliia USENKO

«09» 04 2024

WORKING PROGRAM OF EDUCATIONAL DISCIPLINE

METHODS FOR DETERMINING THE STRUCTURE OF CHEMICAL COMPOUNDS
AND MATERIALS
for students

branch of knowledge **10 Natural Sciences**
specialty **102 Chemistry**
educational level **Master**
educational program **Chemistry**
type of discipline **obligatory**

The form of study **full-time**
Academic year **2024/2025**
Semester **II, III**
Number of ECTS credits **9**
Language of teaching,
learning and assessment **English /Ukrainian**
Final control form **assessment**

Teachers (lecturers)

Pivovarenko Vasyl Georgiovych
Roik Oleksandr Sergiovych
Alekseev Seghij Oleksandrovych
Terebilenko Kateryna Volodymirivna
Vretik Lyudmyla Oleksandrivna

Prolonged:

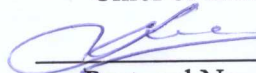
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KYIV – 2024

Developers: Pivovarenko Vasyl Georgiovych
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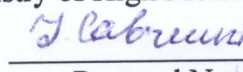
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Chief of Inorganic Chemistry Chair


Rostyslav LAMPEKA
Protocol No. 8 dated March, 2024
13

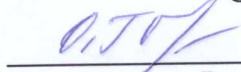
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Chief of Chemistry of High Molecular Compounds Chair


Iryna SAVCHENKO
Protocol No. 11 dated April, 2024
10

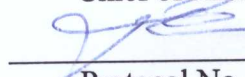
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Chief of Organic Chemistry Chair


Oleksandr GR. YGORENKO
Protocol No. 15 dated March, 2024
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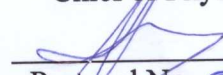
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Chief of Analytical Chemistry Chair


Oksana TANANAİKO
Protocol No. 8 dated March, 2024
28

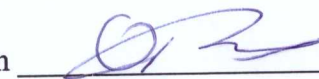
«APPROVED»

Chief of Physical Chemistry Chair


Ihor FRITSKY
Protocol No. 9 dated March, 2024
06

Approved by the scientific and methodical commission of the Chemistry Department

Protocol No. 8 dated April, 2024
9

Chairman of the scientific and methodical commission  Oleksandr ROİK

« 9 » April 2024

1. The goal of the discipline is to learn the main theoretical principles of the set of methods for determining the structure of chemical compounds and materials, namely: fluorescence spectroscopy, scanning electron and transmission microscopy, X-ray spectroscopy of crystalline materials, methods of studying structural and sorption parameters, ionization and molecular weight estimation of nonvolatile, unstable, with high molecular weight organic compounds. Formation of a theoretical basis for understanding the principles of application, advantages, disadvantages, and limitations of the mentioned methods. Formation of practical skills that allow you to combine theoretical knowledge with the study of the structure of chemical compounds and materials, and make a choice of optimal research methods depending on the object and purpose.

2. Prerequisites for mastering or choosing an academic discipline

This course is based on knowledge of courses in the chemistry of high molecular weight organic compounds, inorganic chemistry, analytical chemistry, organic chemistry, and physical chemistry. Successful completion of the specified discipline requires knowledge from courses in higher mathematics, physics, stereochemistry, and quantum chemistry.

3. Abstract of the academic discipline

The presented educational discipline "Methods for determining the structure of chemical compounds and materials" gives students the theoretical foundations and examples of the application of many experimental methods: fluorescence spectroscopy, scanning electron and transmission microscopy, X-ray spectroscopy of crystalline materials, methods of studying structural and sorption parameters, ionization and molecular weight estimation of compounds including nonvolatile, unstable, with high molecular weight. Approaches to the analysis and interpretation of experimental information obtained using the specified research methods are studied. Advantages and limitations of modern methods of studying the structure of compounds and materials are explained.

4. Tasks (learning objectives):

- to form the conception of the physical content and nature of the phenomena that underlie the considered methods of studying the structure of chemical compounds and materials - fluorescence spectroscopy, scanning electron and transmission microscopy, X-ray spectroscopy of crystalline materials, methods of studying structural-sorption parameters, ionization and molecular weight estimation of organic compounds, including nonvolatile, unstable, with high molecular weight;
- to acquaint students with examples of the application of these methods for the study of various compounds and materials;
- to provide the necessary theoretical basis for the application of the methods, as well as an understanding of the advantages, disadvantages, and limitations of the considered methods.

The course «Methods of determining the structure of chemical compounds and materials» is aimed at achieving the following general and professional competencies: 3K1, 3K4, 3K7, 3K10, 3K14, ФK4, ФK6, ФK9

5. Learning outcomes by discipline:

Code	Learning outcome	Forms of teaching and learning	Evaluation methods: current control (activity during practical work ПтК-1, and control of individual work ПтК-2), final control Иск	Percentage in the final grade in the discipline
1.1	To know the mechanisms of occurrence and quenching of fluorescence of chemical compounds, understand the formation of electromotive forces and the nature of the electrode potential	lectures, practical work, individual work	ПтК-1, ПтК-2, Иск	10

1.2	To know and understand the basics of luminescence spectroscopy, factors that affect the splitting, intensity, and width of spectral lines, principles of sensitized luminescence, and mechanisms of non-radiative intramolecular energy transfer.	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	10
1.3	To understand the theoretical foundations of X-ray phase and X-ray structural methods. To know their advantages and limitations when studying crystalline materials.	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	10
1.4	To know the physical methods used to measure the structural sorption parameters of materials and the sizes of nanoparticles, and which calculation models are used for the interpretation of their results	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	10
1.5	Students should know the theoretical foundations of methods of ionization of chemical compounds - FD, FAB, SIMS, MALDI. They should also understand the advantages and disadvantages of these methods in the case of high molecular weight compounds.	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	10
2.1	To use acquired knowledge and skills to interpret experimental information obtained using the considered research methods.	lectures, practical work, individual work	ПтК-2, ПтК-3	10
2.2	Students should be oriented in modern methods of studying the structure of compounds and materials, and be able to choose the optimal method for performing a specific practical task.	Lectures, practical work, and individual work	ПтК-1, ПтК-2, ПсК	10
2.3	They should be able to use acquired knowledge for calculations and modeling of the structure of chemical compounds and materials.	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	10
3.1	The ability to use modern information and communication technologies in communication, as well as to collect, analyze, process, and interpret information related to the study of the structure of substances.	Lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	5
3.2	Ability to perform the tasks provided by the education program in cooperation with other performers	lectures, practical work, individual work	ПтК-1, ПтК-2, ПсК	5
4.1	Be able to independently interpret the results of the experimental methods considered in the course	practical work, individual work	ПтК-2, ПсК	5
4.2	Comply with safety regulations and carry out professional activities with the least risks for the environment	practical work, individual work	ПтК-2, ПсК	5

6. Correlation of discipline learning outcomes (DLU) with program learning outcomes (PLO):

PLO \ DLU (code)	1.1	1.2	1.3	1.4	1.5	2.1	2.2	2.3	3.1	3.2	4.1	4.2
P1. To know and understand the scientific concepts and modern theories of chemistry, as well as the fundamental foundations of related sciences.	+	+	+	+	+							
P2. Deeply understand the basic facts, concepts, principles, and theories related to the subject area mastered during the master's program, use them to solve complex tasks and problems, as well as realize research in the relevant field of chemistry.	+	+	+	+	+	+	+	+				
P3. Apply the acquired knowledge and understanding to solve new qualitative and quantitative problems of chemistry.	+	+	+	+	+	+	+	+				
P4. Be able to synthesize chemical compounds with specified properties, analyze them and evaluate compliance with specified requirements.					+				+	+		
P5. To know the methods of computer modeling of the structure, parameters, and dynamics of chemical systems.				+	+	+	+	+				
P7. Communicate freely in English and (if possible) another foreign language on professional matters, orally and in writing, present the results of research in chemistry in a foreign language, and participate in discussions of chemistry problems.	+	+	+	+	+	+	+	+				
P9. Collect, evaluate, and analyze the data needed to solve complex chemistry problems using appropriate methods and data tools.			+	+	+	+	+	+	+		+	
P10. Plan, organize, and carry out experimental research in chemistry using modern equipment, competently process their results, and draw reasonable conclusions.					+	+	+	+	+	+	+	+
P14. Interpret experimentally obtained data and correlate them with relevant theories in chemistry.						+	+	+	+	+	+	+

7. Scheme of formation of assessment

7.1. Assessment forms.

Semester assessment:

The maximum/minimum number of points that can be obtained by a student: **100 points /60 points**, namely:

1. Modular control work 1: PH 1.1, PH 1.2, PH 1.3, PH 1.4, PH 1.5 – **15/9 points**.
2. Modular control work 2: PH 1.1, PH 1.2, PH 1.3, PH 1.4, PH 1.5 – **15/9 points**.
3. Practical work: PH 2.1, PH 2.2, PH 2.3 – **40/9 points**.
4. Search of literary sources: PH 2.1, PH 2.2, PH 2.3, PH 3.2, PH 4.1 – **30/9 points**

7.2. Evaluation organization:

Assessment deadlines:

Modular control work 1: no earlier than the 8th week of the semester;

Modular control work 2: no earlier than the 13th week of the semester;

Practical work: performed during the whole semester.

Students receive personal tasks for writing a literary search no later than 8 weeks before the end of the semester;

Evaluation of independent work: throughout the semester.

A literature search requires that students conduct an analysis of the literature on the uniqueness of the method of investigation, determine the advantages and disadvantages of the given method, propose methods for confirming the structure of the selected compound or material, and defend the generalized material.

7.3. Rating correspondence scale

Excellent	90-100
Good	75-89
Satisfactory	60-74
Fail	0-59

8. The structure of the academic discipline.
Thematic plan of lectures and practical classes

№ of lecture	Title of lecture	Number of hours		
		Lectures	Practical classes	Individual work
CONTENT MODULE I " Флуоресцентна спектроскопія у дослідженні хімічних сполук та їх розчинів"				
1	Флуоресцентна спектроскопія у стаціонарних умовах. Механізми гасіння флуоресценції. Агрегація сполук у збудженому стані.	2	4	12
2	Часово-розділена флуоресцентна спектроскопія. Міжмолекулярне та внутрішньо молекулярне фото перенесення електрону та внутрішньо молекулярне фотоперенесення заряду.	2	4	12
3	Резонансне перенесення енергії збудження. Внутрішньомолекулярне фотоперенесення протону.	2	4	12
CONTENT MODULE II " Electron Microscopy basics"				
4	Electron Microscopy -Definition, Principle, Types and Application/ Електронна мікроскопія: визначення, принцип роботи, класифікація та використання	2	4	12
5	The core contribution of transmission electron microscopy to functional materials engineering: cryoEM/ Визначальний внесок трансмісійної електронної мікроскопії в інженерію функціональних матеріалів:кріоелектроннамікроскопія	2	4	12
6	Scanning Transmission Electron Microscopy for Materials Science: Imaging, Diffraction, Spectroscopy, and Tomography(STEM)/ Сканувальна просвічуюча електронна мікроскопія для потреб матеріалознавства: принцип роботи, дифракція, спектроскопія та томографія	2	2	12
	Modular control work 1		2	
CONTENT MODULE III " X-ray diffraction analysis of crystalline materials"				
7	Generation of X-ray radiation: X-ray tubes, microfocus X-ray tubes, and synchrotron radiation generation. Monochromatization and detection of X-rays. Basic components of an X-ray diffraction equipment.	2	4	12
8	The Bragg's equation. Family of lattice planes (Miller indices). Using the concept of a reciprocal lattice for the study of crystals. Ewald sphere construction, Crystal structure determination: relationship between d-spacing and lattice constants for various crystal lattices.	2	4	12
9	X-ray powder diffraction method in materials research: qualitative and quantitative phase analysis. Fundamentals of the single-crystal X-ray diffraction technique. X-ray diffraction analysis of macromolecular structures.	2	4	12
CONTENT MODULE IV "Дослідження наноструктурованих матеріалів"				
10	Параметри наноструктурованих матеріалів та фізикохімічні явища, що відбуваються при адсорбції парів. Що таке наноструктуровані матеріали і навіщо їх досліджувати? Питома поверхня, об'єм пор та розподіл пор за розмірами. Фрактальна розмірність. Специфічна та	2	4	12

	неспецифічна адсорбція. Адсорбція парів: рівняння Ленгмюра та БЕТ. Явище капілярної конденсації: рівняння Кельвіна. Класифікація пор за розмірами: мікро-, мезо, та макропори.			
11	Методи дослідження структурно-сорбційних параметрів. Критерії вибору адсорбату для структурно-сорбційних досліджень. Ізотерми адсорбції азоту. Класифікація ізотерм за ІЮПАК. Мезопористі адсорбенти та метод ВЈН. Критерії наявності мікропор в адсорбентах: метод t-plot. Методи розрахунку розподілів мікропор за розмірами. Ртутна порометрія – метод дослідження макропор.	2	4	12
12	Оптичні методи дослідження наночастинок. Явище світлорозсіювання. Рівняння Релея. Метод динамічного світлорозсіювання: фізичні основи, математичне наближення, можливості та обмеження. Вимірювання зета-потенціалу. Метод лазерної дифракції.	2	4	12
CONTENT MODULE V " Методи іонізації високомолекулярних сполук "				
13	Ionization methods of organic molecules - FD, FAB, SIMS and MALDI. Advantages and disadvantages of the ionization methods in a case of polymer ionization. The matrix as a key point in MS spectrometry of high molecular weight compounds.	2	4	12
14	The time-of-flight (TOF) analyzer: linear, with reflection. MALDI spectra, a basic equation to convert the TOF spectrum into a mass spectrum.	2	4	12
15	Cationization agents. Experimental conditions (laser power, cationization agent, and sample polydispersity) and quality of polymer MS spectrum.	2	2	12
	Modular control work 2			
	Total	30	60	180

Totally - **270 hours, including :**

Lectures – **30 hours.**

Practical work – **60 hours**

Individual work - **180 hours.**

Literature

Basic:

1. Ophus, C. (2023). Quantitative Scanning Transmission Electron Microscopy for Materials Science: Imaging, Diffraction, Spectroscopy, and Tomography. *Annual Review of Materials Research*, 53.
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Additional:

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2. •Vernon-Parry, K. D. (2000). Scanning electron microscopy: an introduction. *III-Vs review*, 13(4), 40-44.
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4. Loew, L. M. Spectroscopic Membrane Probes. Boca Raton, CRC Press. 1988. 297 P.
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7. D. Altschuh, S. Oncul and A. P. Demchenko. Fluorescence sensing of intermolecular interactions and development of direct molecular biosensors. *Review. J. Mol. Recognit.* 2006; 19: 459–477.
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9. В.Г. Пивоваренко. "Синтез, будова і властивості багатоканальних флуоресцентних зондів на основі 1,3-діариліденкетонів, дициклопентано[b,e]піридинів та 3-гідроксикхромонів. Дисертація на здобуття наукового ступеня доктора хімічних наук. Київ, Київський національний університет імені Тараса Шевченка, 2007, 580 с.
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