TARAS SHEVCHENKO NATIONAL UNIVERSITY OF KYIV

FACULTY OF CHEMISTRY

«APPROVED»
Deputy dean for academic work
_________ Nataliia USENKO
«30» 06 2022

WORKING PROGRAM OF EDUCATIONAL DISCIPLINE

METHODS OF STRUCTURE CHARACTERIZATION 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 **2022/2023**
Semester **I, II**
Number of ECTS credits **9**
Language of teaching, learning and assessment **English**
Final control form **assessment, exam**

Teachers (lecturers) **Vasyl Pivovarenko**
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Prolonged: for 20__/20__a.y.__________(________) «__»________ 20____
for 20__/20__a.y. _________(_________) «__»________ 20____

KYIV – 2022

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Protocol No. 7 dated June 29, 2022

Chairman of the scientific and methodical commission _____________ Oleksandr ROIK

« 29 » June 2022

1. **The goal of the discipline** is to learn the main theoretical principles of the set of methods for structure characterization of chemical compounds and materials, namely: fluorescence spectroscopy, metal-centered luminescence, X-ray diffraction for crystalline materials, methods of studying structural and sorption parameters characterization and ionization of 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 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 a number of experimental methods: fluorescence spectroscopy, metal-centered luminescence, X-ray spectroscopy of crystalline materials, methods of studying structural and sorption parameters and ionization of compounds. 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 a 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, metal-centered luminescence, X-ray diffraction of crystalline materials, methods of studying structural-sorption parameters characterization and ionization of compounds;
- 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: ЗК1, ЗК4, ЗК7, ЗК10, ЗК14, ФК4, ФК6, ФК9

5. Learning outcomes by discipline:

Code	**Learning outcome**	**Forms of teaching and learning**	**Evaluation methods**: current control (activity during practical work **CC-1** and control of individual work **CC-2**), final control **FC**	**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	CC-1, CC-2, FC	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	CC-1, CC-2, FC	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	CC-1, CC-2, FC	10
1.4	To know the physical methods used to measure the structural sorption parameters of materials and the sizes of nanoparticles, and calculation models which are used for interpretation of their results	lectures, practical work, individual work	CC-1, CC-2, FC	10
1.5	Students should know the theoretical foundations of methods of ionization of chemical compounds - FD, FAB, SIMS, MALDI. They also should understand the advantages and disadvantages of these methods in the case of high molecular weight compounds.	lectures, practical work, individual work	CC-1, CC-2, FC	10
2.1	To use an acquired knowledge and skills to interpret experimental information obtained using the considered research methods.	lectures, practical work, individual work	CC-1, CC-2, FC	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, individual work	CC-1, CC-2, FC	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	CC-1, CC-2, FC	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	CC-1, CC-2, FC	5
3.2	Ability to perform the tasks provided by the education program in cooperation with other performers	lectures, practical work, individual work	CC-1, CC-2, FC	5

4.1	Be able to independently interpret the results of the experimental methods considered in the course	practical work, individual work	CC-1, CC-2, FC	5
4.2	Comply with safety regulations and carry out professional activities with the least risks for the environment	practical work, individual work	CC-1, CC-2, FC	5

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

DLU (code) / **PLO**	**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, 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.					+	+	+	+	+	+	+	+

DLU (code) / PLO	1.1	1.2	1.3	1.4	1.5	2.1	2.2	2.3	3.1	3.2	4.1	4.2
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: **60 points /36 points,** namely**:**

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

Final assessment (in the form of an exam):

The maximum/minimum number of points that can be obtained by a student: **40 points /24 points**.

Learning outcomes that will be evaluated: PH 1.1, PH 1.2, PH 1.3, PH 1.4, PH 1.5.

Form of exam: written work.

Types of tasks: 5 theoretical questions (8 points of each one).

To get a positive grade in the discipline, the exam grade cannot be less than 24 points.

A student is admitted to the exam if during the semester he scored at least 36 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 entire 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

№	Title of lecture	Number of hours		
		Lectures	Practical classes	Individual work
CONTENT MODULE I " Fluorescence spectroscopy in the study of chemical compounds and their solutions "				
1	Fluorescence spectroscopy in stationary conditions. Mechanisms of fluorescence quenching. Aggregation of compounds in the excited state.	2	4	12
2	Time-resolved fluorescence spectroscopy. Intermolecular and intramolecular phototransfer of an electron and intramolecular phototransfer of a charge.	2	4	12
3	Resonance transfer of excitation energy. Intramolecular proton phototransfer.	2	4	12
CONTENT MODULE II " Metal-centered luminescence"				
4	Specificity of luminescence. Classification of luminescence processes depending on the method of excitation of emitting particles. Spontaneous luminescence. Peculiarities of intracentric (metal-centered) luminescence. Molecular terms for lanthanide (III) compounds. Luminescence spectra and luminescence excitation spectra of lanthanide(III)-containing compounds	2	4	12
5	Mechanisms of luminescence quenching processes of the central lanthanide ion for coordination compounds. Luminescence lifetime and luminescence quantum yield and methods of their quantification. Yablonsky diagram in the case of lanthanide coordination compounds: singlet and triplet states, internal conversion, intersystem crossing, nonradiative transitions.	2	4	12
6	Electron-vibrational structure of luminescence spectra and luminescence excitation spectra as a method of evaluating the mode of coordination of ligands. The connection between the Stark structure of the luminescence spectra of coordination compounds of europium and the symmetry of the nearest environment of the central atom	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, 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 quantative phase analysis. Fundamentals of the single-crystal X-ray diffraction technique. X-ray diffraction analysis of macromolecular structures.	2	4	12
CONTENT MODULE IV "Characterization of the nanostructured materials "				
10	What are the nanostructured materials and which for they should be	2	4	12

	studied? Specific surface area, pore volume and pore size distribution. Fractal dimension. Specific and non-specific adsorption. Adsorption of vapors. Langmuir and BET equations. The phenomenon of capillary condensation: Kelvin equation. Classification of the pores by size: micro-, meso- and macropores.			
11	Methods of structure-sorption parameters determination. Criteria of the adsorbate choice for structure-sorption studies. Nitrogen adsorption isotherms. IUPAC isotherms classification. Mesoporous adsorbents and BJH method. Criteria of the micropores presence: t-plot method. Methods of the micropores size distribution calculation. Mercury porosimetry – a methods of macropores study.	2	4	12
12	Optical methods of the nanoparticles study. The phenomenon of light scattering. Raileigh equation. Dynamic light scattering method: physical principle, mathematical approaches, possibilities and limits. Measurements of zeta-potential. Laser diffraction method.	2	4	12
CONTENT MODULE V " Методи іонізації високомолекулярних сполук "				
13	Методи іонізації високомолекулярних сполук - методи FD, FAB, SIMS, MALDI. Переваги та недоліки цих методів у випадку високомолекулярних сполук. Роль матриці в одержанні мас-спектра високомолекулярної сполуки	2	4	12
14	Принцип роботи детектора TOF – лінійного та з рефлектроном, різниця в **MALDI** спектрах, формула залежності дрейфу від співвідношення маса/заряд.	2	4	12
15	Правила підбору катіонізуючого агента Умови одержання коректного мас-спектра полімерів – вплив різних факторів.	2	2	12
	Modular control work 1		2	
	Усього	30	60	180

Totally - **270** *hours., including* :
Lectures – ***30*** *hours.*
Practical work – **60** hours
Individual work **-** ***180*** *hours.*

Literature

Basic:

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Additional:

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Інтернет ресурси

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