**TARAS SHEVCHENKO NATIONAL UNIVERSITY OF KYIV**

**CHEMICAL DEPARTMENT**

**«APPROVED»**
Deputy dean for academic work
_____ Nataliia USENKO
«__» 06. 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 | **part-time** |
| Academic year | **2024/2025** |
| Semester | **I** |
| Number of ECTS credits | **9** |
| Language of teaching, learning and assessment | **English /Ukrainian** |
| Final control form | **assessment** |

Teachers (lecturers)

**Roik Oleksandr Sergiovych**
**Alekseeev Seghij Oleksandrovych**
**Terebilenko Kateryna Volodymirivna**

Prolonged: for 20__/20__a.y._____(_____) «__»_____ 20____

for 20__/20__a.y. _____(_____) «__»_____ 20____

**KYIV – 2024**

Developers: Roik Oleksander Sergiovych
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Protocol No. 9 dated March 6 2024

Approved by the scientific and methodical commission of the Chemistry Department

Protocol No. 9 dated 9. 04, 2024
Chairman of the scientific and methodical commission _____ Oleksandr ROIK

« 9 » 04 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, 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 several experimental methods: fluorescence spectroscopy, scanning electron and transmission microscopy, X-ray spectroscopy of crystalline materials, methods of studying structural and sorption parameters, and ionization of compounds. Approaches to analyzing and interpreting experimental information obtained using the specified research methods are studied. The advantages and limitations of modern methods for 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 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 **ПтК-1,** and control of individual work **ПтК-2**), final control **ПсК** | 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, ПсК | 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 an 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, and 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 risk to the environment | practical work, individual work | ПтК-2, ПсК | 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 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2. Здатність вчитися і оволодівати сучасними знаннями | + | + | + | + | + | | | | | | | | |
| ЗК3. Здатність до абстрактного мислення, аналізу та синтезу. | + | + | + | + | + | + | + | + | | | | | |
| ЗК 6. Здатність генерувати нові ідеї (креативність). | + | + | + | + | + | + | + | + | | | | | |
| ЗК.10. Здатність спілкуватися англійською та (за можливості) іншою іноземною мовою, як усно, так і письмово | | | | | + | | | | + | + | | | |
| ЗК 14. Здатність до пошуку, критичного аналізу та обробки інформації з різних джерел. | | | | + | + | + | + | + | | | | | |
| ФК1. Здатність використовувати закони, теорії та концепції хімії у поєднанні із відповідними математичними інструментами для опису природних явищ. | + | + | + | + | + | + | + | + | | | | | |
| ФК 2. Здатність будувати адекватні моделі хімічних явищ, досліджувати їх для отримання нових висновків та поглиблення розуміння природи, в тому числі з використанням методів молекулярного, математичного і комп'ютерного моделювання . | | | + | + | + | + | + | + | + | | + | | |

**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 11th 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**

| | |
|---|---|
| **Pass** | **60-100** |
| **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 " Electron Microscopy basics"*** | | | | |
| 1 | **Lecture.** Electron Microscopy -Definition, Principle, Types and Application/ Електронна мікроскопія: визначення, принцип роботи, класифікація та використання | 2 | | 20 |
| 2 | The core contribution of transmission electron microscopy to functional materials engineering: cryoEM/ Визначальний внесок трансмісійної електронної мікроскопії в інженерію функціональних матеріалів:кріоелектроннамікроскопія | | | 30 |
| 3 | 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 | | 30 |
| 4 | **Lecture.** Solid-State Fluorescent Inorganic Solids for Visual Detection and LED application. Твердотільні флуоресцентні неорганічні тверді речовини для візуального виявлення та застосування зі світлодіодами. | 2 | 4 | 20 |
| | **Modular control work 1** | | | |
| ***CONTENT MODULE II " X-ray diffraction analysis of crystalline materials"*** | | | | |
| 5 | 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 | | 20 |
| 6 | 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 | | 20 |
| 7 | 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. | | | 20 |
| ***CONTENT MODULE IV "Дослідження наноструктурованих матеріалів"*** | | | | |
| 8 | 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 неспецифічна адсорбція. Адсорбція парів: рівняння Ленгмюра та БЕТ. Явище капілярної конденсації: рівняння Кельвіна. Класифікація пор за розмірами: мікро-, мезо, та макропори. | 2 | | 20 |
| 9 | Методи дослідження структурно-сорбційних параметрів. Критерії вибору адсорбату для структурно-сорбційних досліджень. Ізотерми адсорбції азоту. Класифікація ізотерм за ІЮПАК. Мезопористі | 2 | 2 | 20 |

| | | | | |
|---|---|---|---|---|
| | адсорбенти та метод BJH. Критерії наявності мікропор в адсорбентах: метод t-plot. Методи розрахунку розподілів мікропор за розмірами. Ртутна порометрія – метод дослідження макропор. | | | |
| 10 | Оптичні методи дослідження наночастинок. Явище світлорозсіювання. Рівняння Релєя. Метод динамічного світлорозсіювання: фізичні основи, математичне наближення, можливості та обмеження. Вимірювання зета-потенціалу. Метод лазерної дифракції. | 4 | 4 | 64 |
| | **Total** | 18 | 8 | 244 |

Totally - **270** *hours, including* :
Lectures – ***18 hours.***
Practical work – **8** hours
Individual work **-244** *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*.
2. •S. Pennycook, "Seeing the atoms more clearly: STEM imaging from the Crewe era to today," Microscopy and Microanalysis, vol. 17; no. S2, pp. 1252-1253, 2011.
3. •O. Krivanek, T. Lovejoy and N. Delby, "Aberration-corrected STEM for atomic-resolution imaging and analysis," Journal of Microscopy, vol. 259, no. 3, pp. 165-172, 2015.
4. •K. Kimoto, K. Nakamura, S. Aizawa, S. Isakozawaand Y. Matsui, "Development of dedicated STEM with high stability," Journal of Electron Microscopy (Tokyo), vol. 56, no. 1, pp. 17-20, 2007.
5. J.R. Lakowicz. Principles of fluorescence spectroscopy. Second edition. Kluwer Academic/Plenum Publishers NY, Boston, Dordrecht, London, Moscow, 1999, 698 P.
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8. Yoshio Waseda, Eiichiro Matsubara, Kozo Shinoda X-Ray Diffraction Crystallography. Introduction, Examples and Solved Problems. Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, Germany, Berlin, 2014


**Additional:**


1. Mohammed, A., & Abdullah, A. (2018, November). Scanning electron microscopy (SEM): A review. In*Proceedings of the 2018 International Conference on Hydraulics and Pneumatics—HERVEX, BăileGovora, Romania*(Vol. 2018, pp. 7-9).

2. •Vernon-Parry, K. D. (2000). Scanning electron microscopy: an introduction.*III-Vs review,13*(4), 40-44.


**Інтернет ресурси**

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http://login.webofknowledge.com/
http://www.nbuv.gov.ua/
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