

## Subject card

|                                             |                                                                                                                                                                                                                                                                                                                                                                                             |                                                          |                                         |                                     |                                                                          |            |     |
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| Subject name and code                       | Monographic lecture - Experimental and theoretical methods in the study of coordination compounds, PG_00206235                                                                                                                                                                                                                                                                              |                                                          |                                         |                                     |                                                                          |            |     |
| Field of study                              | Chemical Business                                                                                                                                                                                                                                                                                                                                                                           |                                                          |                                         |                                     |                                                                          |            |     |
| Date of commencement of studies             | February 2026                                                                                                                                                                                                                                                                                                                                                                               |                                                          | Academic year of realisation of subject |                                     | 2026/2027                                                                |            |     |
| Education level                             | Master's studies                                                                                                                                                                                                                                                                                                                                                                            |                                                          | Subject group                           |                                     | Obligatory subject group in the field of study<br>Optional subject group |            |     |
| Mode of study                               | full-time studies                                                                                                                                                                                                                                                                                                                                                                           |                                                          | Mode of delivery                        |                                     | at the university                                                        |            |     |
| Year of study                               | 2                                                                                                                                                                                                                                                                                                                                                                                           |                                                          | Language of instruction                 |                                     | Polish<br>Polish                                                         |            |     |
| Semester of study                           | 3                                                                                                                                                                                                                                                                                                                                                                                           |                                                          | ECTS credits                            |                                     | 3.0                                                                      |            |     |
| Learning profile                            | academic                                                                                                                                                                                                                                                                                                                                                                                    |                                                          | Assessment form                         |                                     | credit                                                                   |            |     |
| Conducting unit                             | Faculty of Chemistry -> Rector                                                                                                                                                                                                                                                                                                                                                              |                                                          |                                         |                                     |                                                                          |            |     |
| Name and surname of lecturer (lecturers)    | Subject supervisor                                                                                                                                                                                                                                                                                                                                                                          |                                                          | dr hab. Joanna Makowska                 |                                     |                                                                          |            |     |
|                                             | Teachers                                                                                                                                                                                                                                                                                                                                                                                    |                                                          |                                         |                                     |                                                                          |            |     |
| Lesson types                                | Lesson type                                                                                                                                                                                                                                                                                                                                                                                 | Lecture                                                  | Tutorial                                | Laboratory                          | Project                                                                  | Seminar    | SUM |
|                                             | Number of study hours                                                                                                                                                                                                                                                                                                                                                                       | 30.0                                                     | 0.0                                     | 0.0                                 | 0.0                                                                      | 0.0        | 30  |
|                                             | E-learning hours included: 0.0                                                                                                                                                                                                                                                                                                                                                              |                                                          |                                         |                                     |                                                                          |            |     |
| Learning activity and number of study hours | Learning activity                                                                                                                                                                                                                                                                                                                                                                           | Participation in didactic classes included in study plan |                                         | Participation in consultation hours |                                                                          | Self-study | SUM |
|                                             | Number of study hours                                                                                                                                                                                                                                                                                                                                                                       | 30                                                       |                                         | 5.0                                 |                                                                          | 40.0       | 75  |
| Subject objectives                          | The aim of the course is to familiarize students with commonly used experimental methods such as potentiometry, conductometry, isothermal titration calorimetry (ITC), and differential scanning calorimetry (DSC) as well as with the theoretical foundations necessary for studying chemical equilibria, designing experiments, performing calculations, and presenting obtained results. |                                                          |                                         |                                     |                                                                          |            |     |

| Learning outcomes | Course outcome                                                                                                                                                                                                                                   | Subject outcome                                                                                                                                                                                                                                                                                                                                                                                            | Method of verification                                                                                                      |
|-------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
|                   | [BCHMU2_W05] Knows and understands the main trends in the development of chemistry combined with economics as two interpenetrating scientific disciplines.                                                                                       | Student knows and understands the possibilities and limitations of modern physicochemical methods, such as microcalorimetry, potentiometry, and conductometry, in the study of chemical systems, and understands the importance of selecting efficient and economically justified analytical methods in the design and implementation of chemical research.                                                | [SW1] oral statement/conversation/discussion<br>[SW3] text preparation/written work                                         |
|                   | [BCHMU2_U01] Is able to, on the basis of her/his knowledge, propose a solution to problems in chemistry, taking into account the economic aspect by using advanced measurement techniques.                                                       | The student is able to select and apply advanced physicochemical methods, such as potentiometry, conductometry, DSC, and ITC, for studying the thermodynamics and equilibria of chemical systems, analyze and interpret the obtained results, and propose solutions to chemical problems while taking into account the cost-effectiveness of the solution and the quality of the performed analyses.       | [SU2] presentation/project/paper/report<br>[SU6] demonstration of practical skills                                          |
|                   | [BCHMU2_U02] Is able to define her/his interests, develop them within the chosen direction and in connection with the subject of her/his master's thesis by implementing the process of self-education and planning her/his professional career. | Student is able to independently develop competencies related to the subject of the implemented project/thesis, search for and analyze specialized information, and plan further academic and professional development.                                                                                                                                                                                    | [SU1] oral statement/conversation/discussion<br>[SU2] presentation/project/paper/report                                     |
|                   | [BCHMU2_K04] Is willing to properly assess the acquired knowledge, respect and disseminate it in order to solve specific cognitive and practical issues.                                                                                         | Student is prepared to critically evaluate results obtained using microcalorimetric methods, potentiometry, and conductometry, properly interpret and present experimental data, and consciously select an appropriate research method for a given problem                                                                                                                                                 | [SK3] text preparation/written work<br>[SK5] implementation of a problem task<br>[SK6] demonstration of practical skills    |
|                   | [BCHMU2_W01] Knows and understands complex physicochemical processes and is able to analyse their course in connection with other fields of science.                                                                                             | Student knows and understands, at an advanced level, the principles and applications of physicochemical methods in the analysis of complex chemical processes, is able to interpret relationships between thermodynamic parameters and the properties of chemical systems, and understands the importance of the economically efficient selection of research methods in chemical and industrial practice. | [SW4] test/exam - oral or written<br>[SW1] oral statement/conversation/discussion<br>[SW5] implementation of a problem task |

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| Subject contents                | <p>Block I: Introduction to Experimental Methods and Chemical Equilibria</p> <p>Fundamentals of thermodynamics of chemical equilibria<br/>Principles of experimental design</p> <p>Block II: Electrochemical Methods Potentiometry</p> <p>Theoretical foundations of potentiometry<br/>Applications in equilibrium studies<br/>Experimental design and data analysis</p> <p>Block III: Electrochemical Methods Conductometry</p> <p>Theoretical foundations<br/>Applications in equilibrium studies<br/>Calculations and data interpretation</p> <p>Block IV: Calorimetric Methods ITC (Isothermal Titration Calorimetry)</p> <p>Principles of ITC<br/>Equilibrium modeling<br/>ITC experimental design<br/>Calculations and presentation of results</p> <p>Block V: Calorimetric Methods DSC (Differential Scanning Calorimetry)</p> <p>Fundamentals of DSC<br/>Determination of equilibrium parameters<br/>Calculations and interpretation of thermograms</p> <p>Block VI: Experimental Design</p> <p>Classical experimental design schemes<br/>Selection of methods for a research problem<br/>Handling errors and measurement uncertainties</p> <p>Block VII: Calculations in Chemical Equilibrium Studies</p> <p>Processing of raw data<br/>Nonlinear modeling<br/>Thermodynamic calculations</p> <p>Block VIII: Presentation of Results and Reporting</p> <p>Preparation of clear graphs<br/>Summary tables of parameters<br/>Preparation of a scientific report/publication</p> |
| Prerequisites and co-requisites | <p>Inorganic Chemistry</p> <p>Coordination Chemistry</p> <p>Analytical Chemistry</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

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| Assessment methods and criteria | Subject passing criteria                                                                                                                                                   | Passing threshold                                                                                                                                                                                                                                                                                                                                                        | Percentage of the final grade |
|                                 | The course is assessed by means of a written examination consisting of mixed questions (multiple-choice and open-ended) covering the topics discussed during the lectures. | 51.0%                                                                                                                                                                                                                                                                                                                                                                    | 100.0%                        |
| Recommended reading             | Basic literature                                                                                                                                                           | Metody instrumentalne w analizie chemicznej, Walenty Szczepaniak. Wydawnictwo: Wydawnictwo Naukowe PWN.                                                                                                                                                                                                                                                                  |                               |
|                                 | Supplementary literature                                                                                                                                                   | 1) Robert de Levie, How to Use Excel® in Analytical Chemistry And in General Scientific Data Analysis, Cambridge University Press (2001)<br><br>2) Jean-Louis Burgot, Ionic Equilibria in Analytical Chemistry, Springer Science+Business Media (2012)<br><br>3) Brian M. Tissue, Basics of Analytical Chemistry and Chemical Equilibria, John Wiley & Sons, Inc. (2013) |                               |
|                                 | eResources addresses                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                          |                               |

Example issues/  
example questions/  
tasks being completed

Block: Introduction and Thermodynamics

- Derive the relationship between the equilibrium constant  $K$  and the standard Gibbs free energy  $\Delta G$ .
- Explain the difference between the thermodynamic equilibrium constant and the concentration-based equilibrium constant.
- Discuss the influence of temperature on the equilibrium constant based on the van t Hoff equation.
- What are the criteria for selecting an experimental method to study a given chemical equilibrium?

Block: Potentiometry

- Explain the role of the reference electrode. Why must its potential be constant?
- Describe how to determine the dissociation constant  $K_a$  of a weak acid using potentiometric titration.

Block: Conductometry

- Why does the molar conductivity of a weak electrolyte decrease with increasing concentration?
- Describe the shape of the conductometric titration curve for the reaction: strong acid + strong base.
- How can the degree of dissociation of a weak electrolyte be estimated from conductometric data?

Block: ITC (Isothermal Titration Calorimetry)

- What three thermodynamic parameters can be obtained from a single ITC experiment?
- Explain the significance of the parameter  $c = nK[M]c = nK[M]$  in designing an ITC experiment.
- How can specific binding be distinguished from nonspecific binding using ITC?

Block: DSC (Differential Scanning Calorimetry)

- What does the abbreviation DSC stand for, and what is the measurement principle?
- Define  $T_m$ ,  $\Delta H_{cal}$ , and  $\Delta C_p$ .
- What is the difference between  $\Delta H_{cal}$  and  $\Delta H_{vH}$  (van t Hoff enthalpy)?
- What might a ratio  $\Delta H_{cal}/\Delta H_{vH} > 1$  indicate?

Problem Questions (Discussion)

- Why is it necessary to maintain constant ionic strength in potentiometric measurements?
- Your ITC data cannot be fitted to a single-site binding model. What are the possible causes?
- In DSC, you observe two endothermic peaks during protein heating. What might this indicate?
- Can conductometry be used to study equilibria in nonpolar solvents? Justify your answer.
- How can you check whether the  $\Delta H$  value obtained from ITC is consistent with that determined by the van t Hoff method (e.g., from potentiometry at different temperatures)?

Sample Calculation Problems Problem 1 (Potentiometry)

In a potentiometric titration of 50.0 mL of a weak acid HA (0.01 M) with NaOH (0.01 M), the pH at half the equivalence point was 4.76. Calculate  $K_a$  and  $pK_a$  of this acid.

Problem 2 (Conductometry)

The limiting molar conductivities  $\Lambda_0$  for HCl, NaCl, and NaOAc are 426, 126, and 91 S·cm<sup>2</sup>/mol, respectively. Calculate  $\Lambda_0$  for HOAc (acetic acid).

Problem 3 (ITC)

In an ITC experiment for binding of ligand L to protein P (1:1 model), the following were obtained:  $n = 1.02$ ,  $K = 2.5 \times 10^5 \text{ M}^{-1}$ ,  $\Delta H = 45 \text{ kJ/mol}$ . Calculate:

- $\Delta G$  (at 298 K)
- $\Delta S$

Problem 4 (DSC)

A DSC thermogram of a protein shows an endothermic peak with  $T_m = 60^\circ\text{C}$  and  $\Delta H_{cal} = 300 \text{ kJ/mol}$ . Assuming a two-state model, calculate  $\Delta S$  and  $\Delta G$  at  $T_m$ .

Problem 5 (Design)

You need to study the complexation of  $\text{Ca}^{2+}$  ions with EDTA (stability constant  $\log K = 10.7$ ). Which method (potentiometry, conductometry, ITC, DSC) is most suitable and why? Propose a concentration range.

|                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
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|                | <p>Self-Check Multiple-Choice Questions (Single correct answer)</p> <p>1. Which method allows simultaneous determination of <math>K_K</math>, <math>\Delta H</math>, and <math>n</math> in a single experiment?</p> <ul style="list-style-type: none"> <li>a) Potentiometry</li> <li>b) Conductometry</li> <li>c) ITC</li> <li>d) DSC</li> </ul> <p>2. In potentiometric titration, the equivalence point is located at:</p> <ul style="list-style-type: none"> <li>a) maximum pH</li> <li>b) steepest slope of the pH vs. volume curve</li> <li>c) minimum potential value</li> <li>d) zero of the second derivative</li> </ul> <p>3. The <math>cc</math> parameter in ITC should fall within the range:</p> <ul style="list-style-type: none"> <li>a) 0.01 0.1</li> <li>b) 1 1000</li> <li>c) 10 500</li> <li>d) <math>&gt; 10</math></li> </ul> <p>4. Differential Scanning Calorimetry (DSC) directly measures:</p> <ul style="list-style-type: none"> <li>a) mass change as a function of temperature</li> <li>b) difference in heat flow between sample and reference</li> <li>c) change in conductivity as a function of temperature</li> <li>d) emission of infrared radiation</li> </ul> |
| Work placement | Not applicable                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |

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