University of Gdańsk

Subject card

Subject name and code	Monographic lecture - Experimental and theoretical methods in the study of coordination compounds, PG_00206234		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2027/2028
Education level	Master’s studies	Subject group	Obligatory subject group in the field of study Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	2	Language of instruction	Polish
Semester of study	4	ECTS credits	3.0
Learning profile	academic	Assessment form	credit
Conducting unit	Department of General and Inorganic Chemistry -> Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Dariusz Wyrzykowski	
	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
	[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	Student possesses advanced knowledge of spectroscopic methods for the analysis of chemical compounds, understands the principles of spectroscopic techniques, and is able to interpret the obtained spectra in order to determine the structure and properties of the studied compounds.	[SW3] text preparation/written work [SW5] implementation of a problem task
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Student understands the limitations of physicochemical methods used in the study of chemical systems, recognizes the need for continuous expansion of knowledge in modern analytical techniques, and is able to independently search for and use scientific information to develop their own competencies.	[SK1] oral statement/conversation/discussion [SK2] presentation/project/paper/report
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student possesses advanced knowledge of physicochemical methods used in the study of equilibria and thermodynamics of chemical systems, in particular potentiometry, conductometry, and microcalorimetric methods (DSC, ITC), and understands their application in the analysis of chemical and industrial problems.	[SW4] test/exam - oral or written [SW1] oral statement/conversation/discussion
	[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	Student demonstrates advanced knowledge of modern research methods used in chemistry and current trends in the development of analytical and physicochemical techniques, understands their importance in the advancement of contemporary chemistry, and is able to apply the latest scientific achievements to the interpretation of chemical processes.	[SW1] oral statement/conversation/discussion [SW2] presentation/project/paper/report

Subject contents	
Subject contents	Block I: Introduction to Experimental Methods and Chemical Equilibria 1. Fundamentals of chemical equilibrium thermodynamics 2. Principles of experiment design Block II: Electrochemical Methods Potentiometry 1. Theoretical foundations of potentiometry 2. Applications in studying equilibria 3. Data design and analysis Block III: Electrochemical Methods Conductometry 1. Theoretical foundations 2. Applications in studying equilibria 3. Calculations and interpretation Block IV: Calorimetric Methods ITC (Isothermal Titration Calorimetry) 1. Principle of ITC operation 2. Equilibrium modeling 3. ITC experiment design 4. Calculations and data presentation Block V: Calorimetric Methods DSC (Differential Scanning Calorimetry) 1. Fundamentals of DSC 2. Determination of equilibrium parameters 3. Calculations and interpretation of thermograms Block VI: Experiment Design 1. Classical design schemes 2. Method selection for a research problem 3. Handling errors and measurement uncertainties Block VII: Calculations in the Study of Chemical Equilibria

	1. Raw data processing 2. Nonlinear modeling 3. Thermodynamic calculations Block VIII: Data Presentation and Reporting 1. Creating clear graphs 2. Summary parameter tables 3. Preparing a scientific report / publication
Prerequisites and co-requisites	Inorganic Chemistry Coordination Chemistry Analytical Chemistry
Assessment methods and criteria	see table below

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) 2) Jean-Louis Burgot, Ionic Equilibria in Analytical Chemistry, Springer Science+Business Media (2012) 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 ΔG.
- 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 KaKa 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 TmTm, ΔHcalΔHcal, and ΔCpΔCp.
- What is the difference between ΔHcalΔHcal and ΔHvHΔHvH (van t Hoff enthalpy)?
- What might a ratio ΔHcal/ΔHvH>1ΔHcal/ΔHvH>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 $\Delta H\Delta H$ value obtained from ITC is consistent with that determined by the van t Hoff method (e.g., from potentiometry at different temperatures)?

Sample Calculation ProblemsProblem 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 $KaKa$ and pKa of this acid.

Problem 2 (Conductometry)

The limiting molar conductivities $\Lambda 0\Lambda 0$ for HCl, NaCl, and NaOAc are 426, 126, and 91 S·cm²/mol, respectively. Calculate $\Lambda 0\Lambda 0$ 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: $n=1.02n=1.02$, $K=2.5\times105M1K=2.5\times105M1$, $\Delta H=45kJ/mol\Delta H=45kJ/mol$. Calculate:

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

Problem 4 (DSC)

A DSC thermogram of a protein shows an endothermic peak with $Tm=60CTm=60C$ and $\Delta Hcal=300kJ/mol\Delta Hcal=300kJ/mol$. Assuming a two-state model, calculate $\Delta S\Delta S$ and $\Delta G\Delta G$ at $TmTm$.

Problem 5 (Design)

You need to study the complexation of $Ca2+Ca2+$ ions with EDTA (stability constant $logK10.7logK10.7$). Which method (potentiometry, conductometry, ITC, DSC) is most suitable and why? Propose a concentration range.

Self-Check Multiple-Choice Questions (Single correct answer)

1. Which method allows simultaneous determination of KK, $\Delta H\Delta H$, and nn in a single experiment?

- a) Potentiometry
- b) Conductometry
- c) ITC
- d) DSC

2. In potentiometric titration, the equivalence point is located at:

- a) maximum pH
- b) steepest slope of the pH vs. volume curve

	• c) minimum potential value • d) zero of the second derivative 3. The cc parameter in ITC should fall within the range: • a) 0.01 0.1 • b) 1 1000 • c) 10 500 • d) > 10 4. Differential Scanning Calorimetry (DSC) directly measures: • a) mass change as a function of temperature • b) difference in heat flow between sample and reference • c) change in conductivity as a function of temperature • d) emission of infrared radiation
Work placement	Not applicable