

PHD STUDIES COURSE UNIT DESCRIPTION

Name of subject	Field of science, code	Faculty / Center	Department
Spectroscopic methods of Analysis	Chemistry N 003	Faculty of Chemistry and Geosciences	Department of Analytical and Environmental Chemistry
Student's workload	Credits	Student's workload	Credits
Lectures		Consultations	2
Independent study	8	Seminars	

Course annotation

Atomic Absorption Spectrometry (AAS). Fundamentals of the method. AAS using flame atomization. Equipment. Radiation sources. Flames and burners. Performance of analysis, sensitivity, main problems and interferences. AAS using electrothermal atomization (graphite cuvette). Performance of analysis. Mechanism of evaporation in graphite cuvette. Application of AAS for the analysis of different types of samples.

Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES). Fundamentals of ICP-OES, main characteristics and application areas. Origin of atomic/ionic emission, qualitative and quantitative analysis. Inductively coupled plasma as an excitation source. Equipment, types of spectrometers, performance of analysis, main advantages and disadvantages. Interferences. Sample preparation. Other excitation sources.

Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Fundamentals of ICP-MS, equipment and types of spectrometers. The role of plasma as an ion source. Sensitivity of ICP-MS. Main advantages and disadvantages, interferences. Performance of analysis and application for different types of samples.

Atomic Fluorescence Spectrometry (AFS). Fundamentals of AFS, main characteristics. Equipment, main advantages and disadvantages.

Molecular Spectroscopy. Fundamentals of optical spectroscopic method, main. Basic concepts. Electronic structure of molecules. Energy levels, energy transitions and corresponding types of spectroscopy

Electronic Absorption Spectroscopy. UV spectra of organic compounds, their structure, information obtained from spectra. Influence of solvent, conjugation and structural changes on the intensity and position of absorption bands. UV spectra of complex inorganic compounds. Absorption bands, their nature. Practical application. Quantitative analysis.

Vibrational Spectroscopy. Principles of methods. Oscillations of molecular bonds, their mathematical description. Infrared spectroscopy. Near, far, main IR radiation areas. Interpretation of IR spectra. Factors influencing the position, width, intensity of absorption peaks. Sample preparation, apparatus and recording techniques. Raman spectroscopy. The essence of the method, the object of research. Information obtained from Raman spectra. Surface-enhanced Raman spectroscopy.

Masių spektrometrija. Techniques and principles. Methods of obtaining of molecular ions. Fragmentation rules and mechanisms, information derived from mass spectra. Combination of mass spectrometry with chromatography. Combination of different analytical methods.

Reading list

1. J. Nolte, ICP Emission Spectrometry; A practical guide, Wiley, 2003.
2. L. Ebdon, E.H. Evans, A. Fisher, S.J. Hill, An introduction to Analytical Atomic Spectrometry, Wiley, 1998.
3. J. A.C. Broekaert, Analytical Spectrometry with Flames and Plasmas, Wiley, 2002.
4. S.M. Nelms, ICP Mass Spectrometry Handbook, Blackwell Publishing, 2005.
5. L.H.J. Lajunen, P. Peramaki, Spectrochemical Analysis by Atomic Absorption and Emission, 2nd edition, The Royal Society of Chemistry, 2004.
6. H. Hesse, A. Meyer, A. Zeeh, Spectroscopic Methods in Organic Chemistry, Thieme, 1997.
7. R. M. Silverstein, F.X. Webster, Spectroscopic identification of Organic Compounds, Wiley, 1997
8. P. Atkins, J. de Paula, "Atkin's Physical Chemistry", 2006.
9. D. Mickevičius „Cheminės analizės metodai“, 1 tomas., 1998
10. R. Kellner, J.M. Mermet, M. Otto, H.H. Widmer, Analytical chemistry, 1998

The names of consulting teachers	Science degree	Main scientific works published in a scientific field in last 5 year period
Stasys Tautkus	Prof.	<p>1. A. Kizalaite, V. Brimiene, G. Brimas, J. Kiuberis, S. Tautkus, A. Zarkov, A. Kareiva, Determination of trace elements in adipose tissue of obese people by microwave-assisted digestion and inductively coupled plasma optical emission spectrometry, <i>Biological Trace Element Research</i> 189 (2019) 10-17.</p> <p>2. L. Sinusaite, I. Grigoraviciute-Puroniene, A. Popov, K. Ishikawa, A. Kareiva, A. Zarkov, Controllable synthesis of tricalcium phosphate (TCP) polymorphs by wet precipitation: effect of washing procedure, <i>Ceramics International</i> 45 (2019) 12423-12428.</p>
Aleksej Žarkov	Dr.	<p>3. P. Konieczynski, A. Zarkov, A. Viapiana, M. Kaszuba, L. Bielski, M. Wesolowski, Investigations of metallic elements and phenolics in Chinese medicinal plants, <i>Open Chemistry</i> 18(1) (2020) 1381-1390.</p> <p>4. L. Sinusaite, A. Popov, E. Raudonyte-Svirbutaviciene, J.-C. Yang, A. Kareiva, A. Zarkov, Effect of Mn doping on hydrolysis of low-temperature synthesized metastable alpha tricalcium phosphate, <i>Ceramics International</i> 47(9) (2021) 12078-12083.</p> <p>5. D. Karoblis, A. Zarkov, E. Garskaite, K. Mazeika, D. Baltrunas, G. Niaura, A. Beganskiene, A. Kareiva, Study of gadolinium substitution effects in hexagonal yttrium manganite $YMnO_3$, <i>Scientific Reports</i> 11(1) (2021) 2875.</p>

Certified during Doctoral Committee session on September 28th, 2021. Protocol No. 610000-KT-142.
Committee Chairman prof. habil. dr. Aivaras Kareiva