PhD STUDIES COURSE UNIT DESCRIPTION

Name of subject	Field of science, code	Faculty / Center	Department
Spectroscopy of organic compounds	Chemistry N 003	Faculty of Chemistry and Geosciences	Departament of Organic Chemistry
Student's workload	**Credits**	**Student's workload**	**Credits**
Lectures		Consultations	3
Independent study	7	Seminars	

Course annotation

Identification of organic compounds applying spectroscopic methods and spectra analysis.
Main methods:
UV/Vis spectroscopy – UV spectra and their structure of organic compounds. Solvent, conjugation, structural changes influence to the absorption curves shape and position. Chiroptical methods: optical rotatory dispersion and circular dichroism;
Vibrational spectroscopy – IR spectra interpretation, stretching and bending vibrations. Factors that influence absorption curves shape, position and intensity. Information from Raman spectra. Surface-enhanced Raman spectroscopy;
Mass spectrometry – ion formation and chemistry. Unimolecular fragmentation and it's mechanism;
NMR spectroscopy – principals, NMR equipment. Chemical shift. Atomic and molecular shielding and deshielding. Anisotropy. Chemical shifts. Signal multiplets. Coupling constant. Chemical and magnetical nuclear equivalence.
Spectral analysis of saturated, unsaturated, aromatic and functionalized organic compounds structures using combination of UV/Vis, IR, Raman, NMR spectroscopy mass spectrometry methods.
Determination of stereo configuration of organic compounds with spectrical methods.
Modern NMR methods in structure determination. First-order and second-order effects in coupling systems. „Tree" diagrams, non-equivalent coupling systems, their analysis. Dynamic processes in NMR spectroscopy. Coalescence temperature and rate constant calculations. Transformations, registering transition state, ketoenol tautomerism, intermolecular proton exchange. Other nuclear (^{11}B, ^{15}N, ^{19}F, ^{31}P etc.) spectroscopy. Various nucleus relaxation times and variation. Shift reagents, chiral shift reagents. Nuclear double resonance experiments (decoupling, saturation etc.), Nuclear Overhauser effect. 2D and 3D NMR spectroscopy. Two-dimensional homonuclear, heteronuclear, NOESY, TOCSY spectra. Structure determination of supramolecules and natural compounds.

Reading list

1. H. Hesse, A. Meyer, A. Zeeh, Spectroscopic Methods in Organic Chemistry, Thieme, 1997.
2. R. M. Silverstein, F.X. Webster, Spectroscopic identification of Organic Compounds, NY, John Willey, 1997
3. P. Atkins, J. de Paula, "Atkin's Physical Chemistry", 2006.
4. Clayden J., Greeves N., Waren S., Wothers P. Organic Chemistry. Oxford, OUP. 2001.
5. H. Friebolin. Basic One- and Two-Dimensional NMR Spectroscopy. Wiley-VCH. 1991.

The names of consulting teachers	Science degree	Main scientific works published in a scientific field in last 5 year period
Ieva Žutautė	Dr.	1. I. Karpavičienė, M. Jonušis, K. Leduskrasts, I. Misiūnaitė, E. Suna, I. Čikotienė, *Dyes and Pigments*, **2019**, 170, 107646. 2. J. Dinić, C. Ríos-Luci, I. Karpaviciene, I. Cikotiene, M. X. Fernandes, M. Pešić, J. M. Padrón, *Invest New Drugs*, **2020**, 38, 584 – 598. 3. T. Javorskis, I. Karpavičienė, A. Jurys, G. Snarskis, R. Bukšnaitienė, E. Orentas, *Angew. Chem. Int. Ed.*, **2020**, 59, 20120– 20128.

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Committee Chairman prof. habil. dr. Aivaras Kareiva