



COURSE UNIT (MODULE) DESCRIPTION

Course unit (module) title	Code
Optical spectroscopy	

Lecturer(s)	Department(s) where the course unit (module) is delivered
Coordinator: Prof. Valdas Šablinskas Others: Prof. Gediminas Niaura Prof. Gerald Steiner	Institute of Chemical Physics

Study cycle	Type of the course unit (module)
II	Compulsory

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Lectures, seminars, laboratory works	II (spring) semester	Lithuanian/English

Requirements for students	
Prerequisites: Knowledge of general physics and quantum mechanics	Additional requirements (if any):

Course (module) volume in credits	Total student's workload	Contact hours	Self-study hours
10	280	96	184

Purpose of the course unit (module): programme competences to be developed		
Learning modern methods of spectroscopy and how to apply them in practice		
Learning outcomes of the course unit (module)	Teaching and learning methods	Assessment methods
Will be able to perform spectroscopic studies using modern FTIR, Raman and SFG spectrometers	Lectures, spectroscopic experiments	Tests (written) and questions/discussion during lectures and written exam
Student will be trained to plan, organize and solve the given problems and provide a summary of main results	Reports, individual work	Evaluation of the reports, discussions
Student will manage to choose right spectroscopic methods in order to understand physical, chemical and biochemical phenomena on molecular level	Lectures, initial phase of report preparation	Analysis of the particular case, questions/discussion during lectures
Student will be able to understand modern methods of modern optical spectroscopy	Optical experiments, report presentation, individual work	Evaluation of the reports, final written exam
Will be able to work in multi scientific teams of physicists, chemists and biologist and apply knowledge in optical spectroscopy	Lectures, optical experiments in different scientific laboratories	Written exam, evaluation of the laboratory work

Content: breakdown of the topics	Contact hours						Self-study work: time and assignments		
	Lectures	Tutorials	Seminars	Exercises	Laboratory work	Internship/work	Contact hours	Self-study hours	Assignments

1. Theoretical foundations of optical spectroscopy. Light absorption and emission. Energy eigenvalues and eigenfunctions of a particle in a potential well; Born-Oppenheimer approximation.	4						4	10	Study of literature, preparation for exercises and laboratory work
2. Recording of optical spectra. Physical principles of spectrum recording. Components of spectroscopic instruments.	4						4	6	Study of literature, preparation for exercises and laboratory work
3. Vibrational energy levels of diatomic molecules. Solution to the Schrödinger equation for a diatomic molecule. Characteristics of distribution of vibrational energy levels.	2						2	8	Study of literature, preparation for exercises and laboratory work
4. Raman scattering. Molecular polarizability.	4						4	6	Study of literature, preparation for exercises and laboratory work
5. Vibrational anharmonicity. Potential functions of real molecules. Dissociation energy. Morse potential.	2						2	6	Study of literature, preparation for exercises and laboratory work
6. Rotational structure of vibrational energy levels. Quantization of rotational energy. Centrifugal distortion.	2						2	6	Study of literature, preparation for exercises and laboratory work
7. Vibrational spectroscopy of polyatomic molecules. Number of degrees of freedom of polyatomic molecule.	4						4	6	Study of literature, preparation for exercises and laboratory work
8. Molecular symmetry and its application in vibrational analysis. Symmetry elements. Point symmetry groups. Symmetry types. Assignment of normal modes to different symmetry types.	10						10	12	Study of literature, preparation for exercises and laboratory work
9. Raman scattering of polyatomic molecules. Polarizability ellipsoid. Depolarization ratio of Raman spectral bands. Placzek's rules.	8						8	14	Study of literature, preparation for exercises and laboratory work
10. Electronic absorption and fluorescence spectroscopy. Electronic energy transitions in molecules. Franck-Condon principle. Kasha's rule.	4						4	6	Study of literature, preparation for exercises and laboratory work
11. Statistical analysis of vibrational spectra. Supervised and unsupervised statistical methods for spectral processing. Cluster analysis. Principal component analysis.	4						4	8	Study of literature, preparation for exercises and laboratory work
12. Fermi resonance. Mechanism, examples, and use for interpretation of vibrational spectra.	2						2	4	Study of literature, preparation for exercises and laboratory work
13. Selection rules in IR and Raman spectra. Physical principles and characteristic band intensities in vibrational spectra.	2						2	4	Study of literature, preparation for exercises and laboratory work
14. Resonance Raman spectroscopy (RRS). RRS instrumentation; sample degradation issues. Raman scattering cross-section. RRS theory; A and B terms. RRS excitation profiles. Anomalous polarization. RRS of heme proteins and blue copper proteins. UV-RRS of the peptide bond. Kinetic UV-RRS.	6		2		4		12	12	Study of literature, preparation for exercises and laboratory work
15. Vibrational spectroscopy of aromatic amino acids and polynucleotides. Spectral markers.	4						4	12	Study of literature, preparation for

Comparison of UV-RRS and non-resonant Raman spectra. Influence of H2O/D2O solvent exchange on the spectra. Interpretation of vibrational spectra of biological macromolecules (viruses, proteins, peptides). Spectrum–structure correlations.									laboratory work
16. Vibrational spectroscopy of carbon derivatives. Resonant Raman spectroscopy of graphene, graphene oxide, carbon nanotubes, and other compounds. Structure of graphene oxide. Influence of defects on graphene spectra. Dispersion of D and 2D modes. Theory of resonant Raman spectroscopy of graphene. Electron-phonon interaction. Vibrational modes of graphite (G, D, C); low-frequency RRS spectrum of graphite. Raman spectroscopy of nanotubes. Raman spectroscopy of diamond-like carbon. Characterization of graphene oxide functional groups using infrared spectroscopy.	4		2		2		8	16	Study of literature, preparation for exercises and laboratory work
17. Surface vibrational spectroscopy. Surface-enhanced Raman spectroscopy (SERS). Surface enhancement mechanisms. Plasmon resonance. plasmonic surfaces, "hot spots." Distance dependence of SERS enhancement. Surface selection rules. TERS and SHINERS methods. Single-molecule SERS. Surface-enhanced IR absorption spectroscopy (SEIRAS). Sum-frequency generation (SFG) spectroscopy. Challenges of spectral analysis. Influence of excitation radiation polarization on spectra. Influence of defects in CH2 chains on spectra. Phase-sensitive SFG spectroscopy, direct detection of the imaginary signal component. SFG of water, surfactants, and biomolecules. Reflection-absorption infrared spectroscopy (RAIRS), selection rules. RAIRS markers of monolayer packing. Polarization-modulation RAIRS (PM-RAIRS).	8		2				10	32	Study of literature, preparation for exercises and laboratory work
18. Interpretation of vibrational spectra. Characteristic vibrations. Spectrum-structure correlations. Investigation of protein secondary structure using vibrational spectroscopy methods. Amide bond vibrations. Secondary structure markers.	4		2		2		8	168	Study of literature, preparation for exercises and laboratory work
Total	48		8		8		96	184	

Assessment strategy	Weight, %	Deadline	Assessment criteria
Grade of final exam	60	End of semester	Answers to three questions (written/oral, discussion) and interpretation of a vibrational spectrum. Assessment covers the level of understanding of vibrational spectroscopy theory; comprehension of the methods, their capabilities, and limitations; understanding of the molecular-level information about the system under study that can be obtained using a specific vibrational spectroscopy method; and the ability to interpret vibrational spectra.
Grade of seminar and written report	20	During semester	Quality of the written report (10–15 pages), structured as a scientific article will be evaluated, specifically assessing the depth of critical analysis regarding the topic.
Grade of laboratory works	20	During semester	Quality of laboratory work performance, conclusions, defense of the work, and answers to questions regarding the laboratory work.

Author	Year of publication	Title	Issue of a periodical or volume of a publication	Publishing place and house or web link
Compulsary reading				
1) J.R. Ferraro, K. Nakamoto	2003	Introductory Raman Spectroscopy		Academic Press, San Diego, 370 p.
2) K. Nakamoto	1997	Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A: Theory and Applications in Inorganic Chemistry		Wiley, New York, 387 p.
3) B.H. Stuart	2004	Infrared Spectroscopy: Fundamentals and Applications		Wiley, Chichester, 224 p.
4) V. Šablinskas, J. Čeponkus	2014	Modernioji virpesinė spektrometrija		Vilnius, 241 p.
5) E.C. Le Ru, P.G. Etchegoin	2009	Principles of Surface-Enhanced Raman Spectroscopy and Related Plasmonic Effects		Elsevier, Amsterdam, 663 p.
6) G. Niaura	2014	Raman Spectroscopy in Analysis of Biomolecules, in Encyclopedia of Analytical Chemistry		Wiley, 34 p.
Optional reading				
1) V. Vaičiškauskas, G. Babonas, Z. Kuprionis, G. Niaura, V. Šablinskas	2008	Paviršiaus Optinė Spektroskopija		TEV, Vilnius, 185 p.
2) M.W. Urban	1993	Vibrational Spectroscopy of Molecules and Macromolecules on Surfaces		Wiley, New York, 384 p.
3) S.A. Olandepo, K. Xiong, Z. Hong, S.A. Asher, J. Handen, I.K. Lednev	2012	UV Resonance Raman Investigations of Peptide and Protein Structure and Dynamics	Chem. Rev., Vol. 112, pp. 2604-2628.	American Chemical Society, Washington, USA
3) D.P. Stommen, K. Nakamoto	1977	Resonance Raman Spectroscopy	J. Chem. Educ., Vol. 54, p. 474.	American Chemical Society, Washington, USA
4) H. Takeuchi	2011	UV Raman Markers for Structural Analysis of Aromatic Side Chains in Proteins	Analytical Sciences, Vol. 27, 1077-1086.	Japan Society of Analytical Chemistry, Tokyo, Japan
5) E.J. Heller, Y. Yang, L. Kocia, W. Chen, S. Fang, M. Borunda, E. Kaxiras	2016	Theory of Graphene Raman Scattering	ACS Nano, Vol. 10, 235-246.	American Chemical Society, Washington, USA
6) L.M. Malard, M.A. Pimenta, G. Dresselhaus, M.S. Dresselhaus	2009	Raman Spectroscopy in Graphene	Phys. Rep., Vol. 473, 51-87.	Elsevier, Amsterdam, The Netherlands