Information sheet for the course
Molecular Spectroscopy

University: *Alexander Dubček University of Trenčín*	
Faculty: *VILA – Glass Joint Centre*	
Course unit code: *MoSp*	**Course unit title:** *Molecular Spectroscopy*
Type of course unit: *optional*	
Planned types, learning activities and teaching methods: *Lecture: 4 hours weekly/52 hours per semester of study; face to face*	
Number of credits: *10*	
Recommended semester: *1. semester in the 1st year (full-time)* *1. semester in the 1st year (full-time)*	
Degree of study: *III. (PhD)*	
Course prerequisites: *none*	
Assesment methods: *A requirement to complete the subject is the successful passing the examination. The examination is in the form of test that consists of 20 questions (in total 100 points). Gradings: Final letter grades will be assigned according to the following total points earned: A 95-100 points, B 90-95 points, C 80-90 points, D 70-80 points, E at least 60 points.*	
Learning outcomes of the course unit: *A student will receive the integral set of knowledge in the field of molecular spectroscopy (advanced and moder methods of molecular spectroscopy) that will be able to apply in his own field of research closely related to the theme of his dissertation. The student will be able to understand the principles and application of particular spectroscopic techniques in the study of materials, particularly glasses and polycrystalline materials.*	
Course contents: 1. *Introduction to molecular spectroscopy. Basic definitions and terms used in spectroscopy. Electromagnetic radiation, interaction of electromagnetic radiation with matter.* 2. *Theoretical background of the spectroscopy (time-independent and time-dependent Schrödinger equation; quantum-mechanical description of energy of states in atoms and molecules; spectral terms; Einstein phenomenological theory of interaction of electromagnetic radiation and matter; shape and spectral-width of spectral bands and intensity of spectral transitions.* 3. *Experimental background of spectroscopic techniques (methods).* 4. *Atomic absorption spectroscopy/spectrometry (theoretical background, instrumentation in AAS), Atomic fluorescence spectrometry.* 5. *Optical atomic emission spectrometry (theoretical background, instrumentation in OAES, e.g. ICP)* 6. *UV-VIS-NIR spectroscopy (theoretical background – Lambert-Beer law; electronic transitions in transition metal ions and rare-earth ions; probability of spectral transitions and intensity of spectral transitions; selection rules; Frank-Condon principle; matrix effect (effect of solvent and matrix) on spectral bands shift; instrumentation).* 7. *Fluorescence spectroscopy (theoretical background and instrumentation, steady-state and time-resolved fluorescence spectroscopy).* 8. *Infrared and raman spectroscopy (theoretical background – rotational, vibrational and vibration-rotation spectra of two-atomic; rotational and vibrational spectra of multi-atomic molecules; instrumentation).* 9. *Magnetic resonance methods (NMR spectroscopy in solution and solid state, EPR spectroscopy – theoretical background – chemical shift, hyperfine structure, g-factor, hyperfine structure, shape and spectral width of spectral band, instrumentation).*	

10. *Solid state NMR (spectrum vs. structure, structural motives, NMR spectra of glasses and polycrystalline materials).*
11. *Spectral methods based on interaction of X-rays with matter (X-ray fluorescence spectrometry – XRF, X-ray photoelectron spectroscopy – XPS; theoretical background and instrumentation).*
12. *Methods that use synchrotron radiation in the study of materials structure (X-ray absorption spectroscopy – X-ray Absorption Near Edge Structure (XANES), Extended X-Ray Absorption Fine Structure (EXAFS)).*
13. *Examples. Practical solution of the structure and spectral properties of selected complex system (glass/polycrystalline material) from the point of view of different spectral techniques (application of different spectral techniques on a selected complex problem).*
14. *Examples. Practical solution of the structure and spectral properties of selected complex system (glass/polycrystalline material) from the point of view of different spectral techniques (application of different spectral techniques on a selected complex problem).*

Recommended of required reading:

V. Milata, P. Segľa, V. Brezová, A. Gatial, V. Kováčik, M. Miglerini, Š. Stankovský, J. Šima, Aplikovaná molekulová spektroskopia. Vydavateľstvo STU v Bratislave, 2008.

S. Miertuš a kol., Atómová a molekulová spektroskopia, Alfa 1991.

P.W. Atkins, Fyzikálna chémia. Bratislava, STU Bratislava, 1999.

J. Solé, L. Bausa, D. Jaques, An Introduction to the Optical Spectroscopy of Inorganic Solids, Wiley 2005.

J.R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd. edition, Springer 2006.

B.H. Suart, Infrared spectroscopy: Fundamentals and Applications, Wiley 2004.

H. Gunther, NMR Spectroscopy: Basic principles, concepts, and applications in chemistry. Chichester: John Wiley & Sons, 1995.

J. Akitt, NMR and Chemistry : An Introduction to Modern NMR Spectroscopy. London: Chapman and Hall, 1992.

M.J. Duer, Solid State NMR Spectroscopy: Principles and Applications, Wiley-Blackwell 2001.

D.C. Koningsberger, R. Prins, X-Ray Absorption: Principles, Applications, Techniques of EXAFS, SEXAFS and XANES, John Wiley & Sons 1987.

Language: *Slovak*

Remarks: *none*

Evaluation history:

A	B	C	D	E	FX

Lecturer: *Ing. Róbert Klement, PhD.*

Last modification: *31. 1. 2014*

Supervisor: *prof. Ing. Marek Liška, DrSc.*