

<b>General Information</b>			
<b>Course name</b>	<b>ÚCHV/MUS/03 Structure Determination - Spectroscopic Methods</b>	<b>ECTS Credits</b>	<b>10</b>
		<b>Semester</b>	<b>winter</b>
<b>Aims</b>			
<p>To teach students to use methods of molecular spectroscopy, mass spectroscopy and magnetic resonance methods for understanding the structure, properties and reactions of chemical compounds.</p>			
<b>Content</b>			
<p>Fundamentals of molecular spectroscopy, mass spectrometry and magnetic methods as powerful tools for structure determination in chemistry.            Ultraviolet and visible spectroscopy. Emission spectroscopy.            Symmetry and group theory. Infrared and Raman spectroscopy.            Mass spectrometry in organic and analytical chemistry and biochemistry.            Nuclear magnetic resonance - NMR. Chemical shift and splitting of signals by spin-spin coupling. Coupling constants. <sup>1</sup>H NMR, <sup>13</sup>C NMR, NMR of other nuclei. Two- and more dimensional NMR. NMR applications. Nuclear quadrupolar resonance - NQR, Electron paramagnetic resonance - EPR. Mossbauer spectroscopy.            Relations between the spectra and structure, properties and reactions of chemical compound. Methods and instruments used for spectra measurements. Combined application of spectral methods for solution of chemical problems.</p>			
<b>Assessment Methods and Criteria</b>			
<p>Written part of the exam:            It consists of 3 tasks:            1. Solving the specified spectrum.            2. Calculating the number and symmetry of vibrations.            3. Resolving the structure of an unknown compound based on combined spectral applications methods.            Each task is rated in the range of 0-20 points, at least 11 points must be achieved per each task.            Oral examination:            Successful answer of 3 questions. Each question is rated in the range 0-20 points, minimum is 11 points for each question.</p>			

**Grading Scale (in %):**

100-91%-A, 90-81%-B, 80-71%-C, 70-61%-D, 60-51%-E, 50-0%-FX

**Grading System:**

The University recognises the following six degrees for the evaluation of the study results:

- a) A – excellent (excellent results) (numerical value 1)
- b) B – very good (above average results) (1.5)
- c) C – good (average results) (2)
- d) D – satisfactory (acceptable results) (2.5)
- e) E – sufficient (results meet the minimum criteria) (3)
- f) FX – failed (requires further work) (4)

**Bibliography**

1. M. Hesse, H. Meier, B. Zeeh: Spectroscopic Methods in Organic Chemistry. Thieme, NY 1997.
2. L.G.Wade, Jr.: Organic Chemistry. Prentice Hall International, Inc. Englewood Cliffs, New Jersey 1995.

