



## COURSE DATASHEET

<b>Semester:</b>	2012/13/2
<b>Course:</b>	Spectroscopic identification of organic compounds
<b>Code:</b>	VEMKOKM522V
<b>Responsible department:</b>	Department of Organic Chemistry
<b>Department code:</b>	MKOK
<b>Responsible instructor:</b>	József Sándor Pap

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### Course objectives:

Educational objectives: During this practical course the student is introduced to the application of IR, NMR, and MS in the identification of organic compounds.

### Course content:

Detailed content of the subject 1. Basic spectral parameters in the NMR method: chemical shift, spin-spin coupling. <sup>1</sup>H-NMR spectra of organic compounds: saturated, cyclic compounds. 2. <sup>1</sup>H-NMR spectra of unsaturated and aromatic compounds. Chemical shifts of protons bonded to heteroatoms. 3. Heteronuclear coupling (<sup>1</sup>H-, <sup>13</sup>C-, <sup>1</sup>H-<sup>31</sup>P) 4. <sup>13</sup>C-, <sup>31</sup>P NMR 5-6. Two dimensional methods 7. Interpretation of unknown spectra. 8. Basic principles of infrared spectroscopy. Utilization of infrared spectroscopy as a tool for a practising organic chemists. Characteristic group frequencies of hydrocarbons. 9. Absorption frequencies of carbonyl compounds. 10. Spectra of alcohols, ethers, amines, amino acids, nitriles, nitro- and nitroso-compounds, organic sulfur compounds. 11. Interpretation of unknown spectra. 12. Basic principles of mass spectrometry. Recognition of the molecular ion. General rules for fragmentation. Rearrangements. Fragmentation of hydrocarbons and hydroxy compounds. 13. Fragmentation of ketones, aldehydes, esters, acids lactones. Spectra of amines, amides, nitriles, nitrocompounds. 14. Spectra of sulfur and halogen compounds, heteroaromatic compounds. Interpretation of unknown spectra. 15. Test.

### Requirements, evaluation and grading:

Requirements: - attendance is compulsory - passing the test a score of 2 or above

### Required and recommended readings:

Silverstein, Webster, Kiemle: Spectrometric identification of organic compounds. Wiley 2005