

UNIVERSITY OF PANNONIA

COURSE DATASHEET

| Semester: | 2016/17/1 |
|-------------------------|---|
| Course: | NMR spectroscopy |
| Code: | VEMKSI4312S |
| Responsible department: | Department of General and Inorganic Chemistry |
| Department code: | МКАК |
| Responsible instructor: | Szabolcs Balogh |
| | |

Course objectives:

To give introductory theoretical and methodological knowledge of the modern liquid phase NMR methods and draw attention to the possible applications.

Course content:

Introduction: the basic phenomena: the nuclear spin, magnetic and angle-momentum, spin quantum number. Interactions involving the nuclear spins in liquid phase. The NMR spectrometer. Excitation methods (hard and soft pulses), the pulse and Fourier transform method. Acquisition: the quadrature detection method, amplitude, shape and phase of the NMR signal. The relaxation phenomenon, methods of measuring T1 and T2 relaxation constants. The common relaxation mechanisms, the spin echo. Through-space interactions: the nuclear Overhauser effect (NOE) and its applications. Through-bond interactions: the scalar coupling, its interpretation and use. First- and second-order spin systems (AX, AX2, AMX and ABX). Sensitivity enhancement: polarization transfer and spectral editing. INEPT and DEPT. Two-dimensional methods: homonuclear correlations. NOESY, TOCSY, COSY and its variants. Two-dimensional heteronuclear correlations: HETCOR, FLOCK. Inverz heteronuclear correlations (HSQC, HMBC) J-spectroscopy (APT, Spin-echo, HOM2DJ). Gradient promoted spectroscopy. Diffusion ordered spectroscopy (DOSY). Heteronuclear NMR spectroscopy: the method of broad band proton decoupling. Basics of 13C, 15N, 29Si and 31P spectroscopies. Case study: cedrenol.

Requirements, evaluation and grading:

Required and recommended readings:

Szalontai Gábor: Egy- és kétdimenziós NMR eljárások a kémiai szerkezetkutatásban, Veszprém, 2003 (jegyzet CD-n)