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Tuesday 29.05.2012 – Friday 01.06.2012. Lecture – 15 h.

Basic Techniques and Applications of Heteronuclear and Two-dimensional NMR

Rationale
The identification of the molecular structure of chemical compounds and the study of their physical and chemical behavior is a major issue for all synthetic chemistry branches. NMR is not only a powerful method for these purposes. NMR methods but may also find application in many borderline areas connecting chemistry with other sciences, allowing e.g. to explore interactions in living bodies, metabolic pathways, drug-receptor interactions, etc.

Objectives
The aim of the course is to teach the PhD-students methods and concepts in the use of modern NMR methods for the identification of molecular chemical substances. They will gain basic knowledge on the experimental techniques to measure NMR spectra and the procedure to elucidate chemical structures from NMR data.

Contents
Basics of heteronuclear NMR spectroscopy of spin-1/2 (^{19}F, ^{31}P, ^{15}N, ^{29}Si) and quadrupolar nuclei (e.g. ^{7}Li, ^{11}B, ^{17}O, ^{27}Al etc), use of special techniques for signal assignment (DEPT), basic approach to understand the functioning of 2D NMR including the application of pulsed field gradients, important types of homonuclear 2D NMR experiments using correlation through bonds and through space, application of heteronuclear correlation techniques for molecular structure elucidation, study of molecular structural dynamics and chemical reaction pathways by 1D and 2D NMR techniques, strategies for structure elucidation using combined NMR techniques.

Learning outcomes:
The PhD-students have an understanding of modern NMR methods**,** can assess the scope and limitations of these methods for the analytical identification of products, are familiar with the strategies involved in the elucidation of molecular structures from advanced NMR techniques, and have experience with the determination of molecular structures of medium sized unknown molecules from NMR data.