KD2060 NMR-spectroscopy 6.0 credits

NMR-spektroskopi

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for KD2060 valid from Autumn 2007

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Chemistry and Chemical Engineering

Specific prerequisites

1. Equivalent to the basic chemistry and mathematics courses at KTH.
2. The Quantum Chemistry and Spectroscopy course (KD2040) or equivalent is strongly recommended.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After the completed course the student must be able to

- explain and calculate both within a classical and a quantum-mechanical model how the one- and two-dimensional NMR spectrum arises in experiments.

- explain and calculate the effect of Fourier transformation on the detected NMR signal.

- identify elements that separate and unify NMR with other spectroscopic methods.

- explain how NMR relaxation is connected to molecular dynamics.

- explain the basic mechanism of NMR imaging and diffusion and predict the results of imaging simple objects.

- identify the spin interactions that influence the NMR data and explain their effect, connect their spectral effects to chemical properties, select suitable combinations of experiments that can best access those.

Course contents

The course starts with analysing simple NMR phenomena (such as the FID - Free Induction Decay - signal) by spins treated classically. The important elements of practical spectroscopy, including the role of Fourier transformation, are discussed. Understanding more complex NMR demands quantum mechanical treatment, the basis of which is learned in next. This part of the course is finished with a computer experiment where the interesting "quantum life" of spins is observed.

After six lectures of introductory theory the applications take over. First, the two most important two-dimensional (2D) NMR methods, COSY and NOESY spectroscopies, are discussed together with some of the related experiments. NMR relaxation, which forms the basis of NOESY spectroscopy, is treated. This part of the course ends with an overview of the structural studies of biomolecules in solution by multidimensional NMR. The theory is completed with an experiment where non-trivial structural problems are analysed and solved in organic molecules as models.

Applications of NMR to dynamical problems come last. Methods based on magnetic field gradients and used for measuring diffusion and flow (as well as for MR imaging) are discussed together with methods for studying chemical exchange. In the other experiments of the course these methods are going to be applied to dynamical and structural questions in some organic, colloid, and polymer systems.

Course literature

J. Keeler; Understanding NMR spectroscopy, Wiley.

Examination

- TEN1 - Examination, 4.5 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory Work, 1.5 credits, grading scale: P, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

Combined written/oral. Instead of the oral examination the students are going to have the opportunity to give their own seminars about selected subjects. Precondition to attending the exam is the acceptance of the reports of the experimental work and homework solutions.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.