universität ulm
Fakultät für Naturwissenschaften, Fachbereich Physik

Announcement

Theoretical Aspects of NMR Spectroscopy

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Content

- Nuclear spin and its Hamiltonian
- Experimental evidence of the (electron and nuclear) Spin
- QM treatment of the nuclear Spin (angular momentum operator, single sates and wave function)
- Time evolution of a single spin
- Introduction of QSM (time evolution of a spin ensemble)
- Introduction of spin interactions (multiple spin systems)
- Introduction of coherences, relaxation and thermal equilibrium
- Excitation and signal detection
- Gradient and space encoding (introduction of the k-space, Imaging)
- Deduction of the NMR Hamilton operator
- Introduction and discussion of NMR interactions (nuclear shielding vs. chemical shift, dipolar coupling, J-coupling, quadrupolar coupling, paramagnetic and knight shift interactions, secular approximations)
- Feature of the FT-NMR experiment (pulses, phases, setup, sampling, FFT, S/N)
- Density Matrix Description of 2D Experiments (2D-COSY, 2D-HETCOR)
- Powder Spectra (chemical shift and quadrupolar coupling)
- Spectral resolution enhancement (magic angle spinning, spinning sidebands, chemical shift, dipolar coupling and quadrupolar coupling)
- The concept of Echo (rotational echo vs. pulse echo)
- Rotor synchronous experiments (pulse sequences)

Prerequisites

Atomic physics, quantum mechanics

Literature

- A. Abragam; Principles of Nuclear Magnetism; Clarendon Press; 1983.
- C.P. Slichter; Principles of Magnetic Resonance. Springer Series in Solid-State Sciences; Springer Berlin Heidelberg; 1996.
- Melinda J. Duer; Introduction to Solid-State NMR Spectroscopy; John Wiley & Sons; 2005.
- Atta-ur-Rahman und M. Iqbal Choudhary; Applications of NMR Spectroscopy; Bentham; 2015.

Teaching Method

Lecture with exercise (5 hours/week)

Details

6 ECTS credits

Lecturer

Dr. Tobias Speidel, Dr. Raiker Witter, Prof. Dr. Volker Rasche