

THEORY AND APPLICATION OF MULTIDIMENSIONAL NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY.

B.NAGY Ottó, Belgium

The aim of the course is to provide working knowledge in detail of the theoretical foundations of multidimensional NMR spectroscopy. Practical applications are illustrated by analyzing modern pulse sequences both in homo- and hetero-nuclear situations.

1. General features of NMR spectroscopy. Vector diagrams. BLOCH equations. FOURIER transform NMR. Two-dimensional (2D) NMR spectroscopy.

2. Basic quantum theory. The SCHRÖDINGER equation.

3. Nuclear spin. Spin operators. Spin algebra. PAULI matrices. Shift operators. Spin space, product space. Tensor products. Rotations. Conventions. Rotation in Cartesian space and spin space. Rotation matrices.

4. Time-evolution of quantum systems. Exponential operators. Unitary transformations. BAKER-CAMPBELL-HAUSDORFF (BCH) formula. The Hamiltonian operator in NMR. The role of rotating frame.

5. Density matrix. Equilibrium density matrix. Density operator. Time-evolution of the density matrix. The Von NEUMANN equation.

6. Product operators. Matrix representation. Expansion of density matrix into orthogonal operators.

7. Spin system AX. Weak coupling and high temperature approximations. NMR spectrum.

8. Phase of NMR signals. Quadrature detection and frequency discrimination. Spin echo. Spin echo sandwich. Attached Proton Test (APT). Polarization transfer by Selective Population Transfer (SPT).

9. Coherence level diagram. Coherence transfer by through-bond and through space mechanisms. Generation of multi-quantum coherence. Coherence transfer pathway. Selection of coherence pathways. Methods of phase-cycling and of field-gradients. The use of 180° pulses.

10. Two-dimensional (2D) experiments. Correlation spectroscopy, COSY (homo- and hetero-nuclear).

11. Variants of COSY. R-COSY. DR-COSY. DQF-COSY. TQF-COSY. MQF-COSY. E-COSY. FOCY. SECSY.

12. Other pulse sequences. INEPT. DEPT. TOCSY (HOHAHA). INADEQUAT.

13. Nuclear Overhauser Effect (NOE). Cross-relaxation NMR: NOESY and ROESY.

14. Multi-quantum (MQ) spectroscopy. 2Q and 3Q spectroscopies.

15. Hetero-nuclear experiments. HSQC. HMQC. Triple-resonance experiments: the case of proteins.

16. NMR of higher dimensions: 3D, 4D.

Termin	Dzień tygodnia	Godzina	Miejsce
04.04.2016	Poniedziałek	8.00 – 10.15 (bez przerwy)	Minicentrum Konferencyjne (Luwr)
05.04.2016	Wtorek	8.00 – 10.15 (bez przerwy)	Minicentrum Konferencyjne (Luwr)
06.04.2016	Środa	8.00 – 10.15 (bez przerwy)	Minicentrum Konferencyjne (Luwr)
07.04.2016	Czwartek	8.00 – 10.15 (bez przerwy)	Minicentrum Konferencyjne (Luwr)
08.04.2016	Piątek	8.00 – 10.15 (bez przerwy)	Minicentrum Konferencyjne (Luwr)