
NMR Spectroscopy of Organic Compounds

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Syllabus

- The vector model
- Pulses, pulse sequences (Spin echo, APT, INEPT)
- Polarization transfer
- Fourier transform, acquisition parameters, processing NMR spectra
- 2D NMR spectroscopy (principle, the most used methods, inverse detection, gradients of magnetic field)
- NOE, NOESY, ROESY
- Solvent signal suppression, shift reagents, derivatization reactions, selective decoupling ...

Problem solving (1D and 2D)

Syllabus

Lesson 1: Introduction, pulse sequences, 1D experiments (spin echo, APT), relaxation

Lesson 2: Selective pulses, selective decoupling, polarization transfer

Lesson 3: Fourier transform, acquisition parameters, processing 1D experiments

Lesson 4: Basic principle of 2D NMR, most common 2D experiments

Lesson 5: Continuation of 2D NMR, gradients of magnetic field, DOSY

Lesson 6: Nuclear Overhauser effect, NOESY, ROESY

Lesson 7: Fluorine, phosphorus, nitrogen, deuterium, solvent suppression

Lesson 8: Dynamic NMR – reaction monitoring, chemical exchange

Lesson 9: Solid-state NMR spectroscopy

Lesson 10: EPR spectroscopy

Problem solving (1D and 2D)

Recommended reading - Czech

NMR spektroskopie pro chemiky

<https://nmr.group.uochb.cz/cs/vyuka>

Buděšínský, Pelnář: UOCHB: Fyzikálně – chemické metody 3: Nukleární magnetická rezonance

Recommended reading - English

- H. Friebolin: *Basic One- and Two-Dimensional NMR Spectroscopy*. 5th edition, Wiley-VCH, Weinheim, 2010. ISBN-13: 978-3527327829
- H. Günther: *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*. 3rd edition, Wiley-VCH, Chichester, 2013. ISBN-13: 978-3527330003
- J. Keeler: *Understanding NMR Spectroscopy*. 2nd edition, John Wiley & Sons, Chichester, 2010. ISBN-13: 978-0470746080
- M. H. Levitt: *Spin Dynamics: Basics of Nuclear Magnetic Resonance*. 2nd edition, John Wiley & Sons, Chichester, 2008. ISBN-13: 978-0470511176
- T. D. W. Claridge: *High-Resolution NMR Techniques in Organic Chemistry*. 3rd edition, Elsevier Science, Oxford, 2016. ISBN-13: 978-0080999869
- D. C. Apperley, R. K. Harris, P. Hodgkinson: *Solid-State NMR: Basic Principles and Practice*. Momentum Press, New York, 2012. ISBN-13: 978-1606503508
- P. J. Hore, J. A. Jones, S. Wimperis: *NMR: THE TOOLKIT: How Pulse Sequences Work*. 2nd Edition, Oxford University Press, Oxford, 2015. ISBN-13: 978-0198703426

Solving NMR spectra:

- L. D. Field, H. L. Li, A. M. Magill: *Organic Structures from Spectra*. 6th edition, John Wiley & Sons, Chichester, 2020. ISBN-13: 978-1119524809
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The exam

- 80% of homework submitted
- Test (written, in person)