

A Primer of NMR Theory with Calculations in Mathematica

By Alan J. Benesi

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Presents the theory of NMR enhanced with Mathematica© notebooks

- Provides short, focused chapters with brief explanations of well-defined topics with an emphasis on a mathematical description
- Presents essential results from quantum mechanics concisely and for easy use in predicting and simulating the results of NMR experiments
- Includes *Mathematica* notebooks that implement the theory in the form of text, graphics, sound, and calculations
- Based on class tested methods developed by the author over his 25 year teaching career. These notebooks show exactly how the theory works and provide useful calculation templates for NMR researchers

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A Primer of NMR Theory with Calculations in Mathematica By Alan J. Benesi Bibliography

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Editorial Review

From the Back Cover

Presents the theory of NMR enhanced with Mathematica© notebooks in a clear and concise manner

A Primer of NMR Theory with calculations in Mathematica© presents the theory of NMR. Enhanced with Mathematica© notebooks that show exactly how the theory is implemented, the book rigorously covers NMR theory. The Mathematica© notebooks augment the book to demonstrate the theory and applications of NMR, as well as provide calculation templates for students and researchers.

Presented in short, focused chapters the book provides a concise exposition of well-defined topics with emphasis on a mathematical description including essential results from quantum mechanics for easy use in predicting and simulating the results of NMR experiments.

A Primer of NMR Theory with calculations in Mathematica© covers:

The NMR spectrometer
The NMR experiment
Classical magnetic dipole in a magnetic field
The Bloch equation(s)
The vector model of NMR
The density operator and density matrix
The Liouville von Neumann equation
Commutation relations of nuclear spin operators
Time independent perturbation theory
Average Hamiltonian theory
The Powder Average
Effects of exchange on liquid state and solid state NMR spectra
The fundamental connection between molecular motion and NMR relaxation times

While it is not necessary to have Mathematica© to gain understanding from this book, it is highly recommend as the reader can go through the theory presented step by step by executing the Mathematica notebooks. Readers can also copy and modify the Mathematica notebooks for assigned homework or for real research problems.

The Mathematica notebooks are particularly powerful. They can be used as teaching tools and as templates for full blown research calculations. The included notebooks are extremely useful for calculation of matrix representations of nuclear spin operators and for calculation of rotations used in solid state NMR. Other notebooks provide a set of powder average angles necessary for solid state spectral simulations as well as demonstrating simulations of solid state powder patterns, effects of exchange on both liquid state and solid state NMR spectra, and for calculating explicit NMR relaxation times that can be compared to experiment.

Alan J. Benesi was Director of the Pennsylvania State University NMR Facility from 1987-2012. He earned his Ph.D. in Biophysics at the University of California, Berkeley, in 1975. He has published many papers related to solid state and liquid state NMR, solid state and liquid state NMR relaxation, and rotational and

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