Dazzling world of spins

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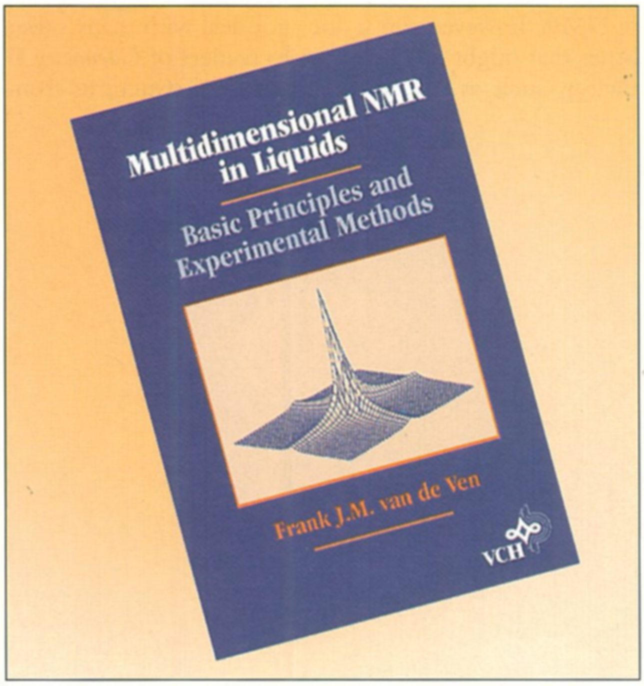
Multidimensional NMR in Liquids: Basic Principles and Experimental Methods by Frank J. M. van de Ven, VCH Publishers, 1995, 399 pages, $55 hardcover (ISBN 1-56081-665-1).



Atomic nuclei are tiny magnets that can feel each other's presence. Over the past few decades, NMR spectroscopists have figured out how to measure these interactions and even more amazingly, how to reconstruct the three-dimensional structure of a macromolecule with this information — by no means a trivial feat.

Compared to his mature and older sister, X-ray crystallography, NMR is the troubled youngster: few understand what drives him, but many are envious of his street-smarts and seemingly bottomless reservoir of tricks. Although there are numerous books on child psychology, they either tend to go into a deep level of psychoanalysis, or provide only a collection of superficial, easy-reading anecdotes. None are written by the little troublemaker himself. Van de Ven's *Multidimensional NMR in Liquids* is the exception.

Next to the now nearly ten year old *Principles of NMR in One and Two Dimensions* by Nobel laureate Richard Ernst and co-workers, van de Ven's book may appear superficial; however, this is not the case. Van de Ven's main 'claim to fame' has been his description of the so-called product operator formalism — simultaneously to the development of the same idea by the Ernst group — for describing the effect of lengthy sequences of radiofrequency pulses on nuclear spins. Next to a rigorous description, this product operator formalism provides some insights in what is actually occurring in the 'dazzling world of spins'. No surprise therefore that van de Ven's book is heavy on product operator formalism. He uses it to take the reader from the simple basis of angular momentum all the way to complex triple resonance experiments on isotopically labeled proteins. This includes some elegant extension of the formalism to the treatment of strongly coupled spin systems (every NMR spectroscopist's nightmare) and analyses of composite pulse decoupling and isotropic mixing schemes.

The book starts with a 50-page introductory chapter which explains in elementary terms what NMR is all about, including simple descriptions of the spectrometer hardware and how it functions, Fourier transformation, and the concept of 'spin coherence'. Also included is a didactic comparison of the description of a spin system in Hilbert and Liouville space. Equally useful to the novice will be the discussion on chemical shifts and the final chapter devoted to nuclear relaxation.

The main purpose of the book is to provide insight into the mechanisms underlying the literally hundreds of different experiments that are now commonly used not only by NMR jocks studying proteins and nucleic acids, but also by hordes of organic and analytical chemists for structure elucidation purposes. Each of these pulse sequences is essentially made up of a subset of roughly a dozen simple building blocks and the author makes a successful attempt at explaining each of these in quite some detail. He illustrates the experiments by applying them to a simple tripeptide, His-Val-Tyr, giving the reader a good feel for the type of information they provide. The DNA-binding domain of bacteriophage Pf3 is used to show the effects of various three-dimensional experiments, including several of the newer variety. A complete set of the experiments in common use today could fill another volume, which would be dated almost immediately as methodological advances in this area outpace the rate at which books can be printed. Instead of selling the reader yesterday's fish, van de Ven is teaching us how to fish today and tomorrow. I therefore do not consider the rather sketchy treatments of four-dimensional NMR, mixed-constant-time experiments, and isotope filtering as major shortcomings. However, I find the absence of more detailed discussions of a popular experiment such as HMBC and solvent suppression techniques such as WATERGATE somewhat disappointing. Another detail which could be improved on is the rather meager index.

The book presumably has grown out of repeatedly teaching the same graduate course over and over again. It discusses complex issues in a language that an ambitious student will be able to follow, even without a solid background in physics or physical chemistry. It also provides an unprecedented view into the spin magician's bag of tricks. The book is restricted to the spectroscopic aspects of NMR, however, and it does not deal with many other issues that might be of interest to readers of *Chemistry & Biology,* such as calculation of protein structures from NMR constraints, and the meaning and interpretation of fuzzy NMR structures. Thus, the book is really intended for those who want to get their hands dirty, and not for the older sister who wants to find out what her delinquent sibling is up to.

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