

Horst Friebolin

Basic One- and Two-Dimensional NMR Spectroscopy

Fourth Completely Revised
and Updated Edition

Translated by
Jack K. Beconsall



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Foreword

Over the past decade, many, if not most, graduate students and postdoctoral fellows in organic chemistry seem to have come to regard nuclear magnetic resonance spectroscopy as a "black box". Something in which you insert an unknown and out comes the data to establish structural formula. Perhaps this trend in the way NMR is perceived is really not surprising, because how manufacturers have tried to package their instruments to be "user friendly" and because of the enormous growth in the sophistication of what NMR instrumentation can do.

Those of us who were fortunate to be in on the beginning of the applications of NMR to organic chemistry in the mid-1950's were able to more or less "grow" with the field and come into the modern arena of multipulse and multidimensional NMR with substantial experience with NMR fundamentals. Those who now wish to start using NMR in their research surely must feel, at least somewhat, overwhelmed by the enormity and sophistication of the currently available knowledge of NMR and must have further concerns at being told by the specialists, that fantastic further, even more sophisticated, developments are in the offing. A "black box" that would function with no need to worry about its inner workings must then be an attractive proposition. The problem is that to properly use modern NMR requires a lot of rather specialized knowledge. The effects of couplings, of exchange, of relaxation times, of low sensitivity, of solvent and so on, make selection of instrumental parameters for taking spectra far from routine. Serious errors or inefficient use of very expensive instrumentation come with ease.

The best way to learn NMR spectroscopy is by doing it, but textbooks, guidebooks and reference books are vitally necessary. Having written two books about NMR basics, with a third in progress, I know something about the difficulties of making available "what every NMR user should know". And it is to this objective that Professor Friebolin has made a wonderfully broad contribution. This book will be of interest and help to both those needing to learn and those needing a reference book to refresh their memories, or extend their capabilities in NMR spectroscopy. It is not a book intended to replace the treatises of Abragam or Bodenhausen, Ernst and Wokaun. However, even though it does start at a useful elementary

level, it goes rather deeply into the difficult basics of multipulse and multidimensional spectroscopy. The result is material that almost every reader will find of value.

The beginner can start with the elements of chemical shifts and couplings and later proceed to more difficult matters. The expert can find ways of explaining what he is doing, without necessarily resorting to density matrices; or else, in impatience with an eager, but dull, learner, can say "Go read about it in Friebolin, then we can talk".

Much is covered in this book in meaningful detail. There is a plethora of structural parameters for proton and carbon NMR and many examples of how they can be used. Best of all, though, are very clear, meticulously written descriptions of INEPT, DEPT, INADEQUATE, COSY, NOESY, and the like, in one- and two-dimensional NMR spectroscopy. Experts may prefer mathematical equations for compactness and "it is easy to see". I prefer descriptions such as those used by Professor Friebolin, which will indeed require careful reading, rereading and drawing and redrawing ones own vector diagrams, but can lead to a real level of understanding. Such understanding in its turn can only result in improved ability to take and interpret NMR spectra.

November 28, 1990

John D. Roberts
Pasadena, California

The Nightingale and the Lark

What can one say to those writers who blithely
fly far above the heads of most of their readers?
The same, surely, as the nightingale said to the
lark: My friend, are you soaring so high in order
that your song cannot be heard?

Gotthold Ephraim Lessing

Preface to the Fourth Edition

Only minor additions were needed for this new edition, at least as far as the fundamentals and methods used in NMR spectroscopy are concerned. Worthy of mention here is the new definition of the δ value in Chapter 1, in accordance with the recommendations of the IUPAC Committee in 2001. Among the many new 2D experiments, I have only incorporated the ROESY Experiment in Chapter 9, since this has now become a routine operation.

Much progress has been made, on the other hand, in explaining the structure of large molecules. I have taken this trend into consideration and expanded Chapter 13 “Macromolecules” by way of a comprehensive section on biopolymers. Since solid state NMR spectroscopy has gained importance in investigating synthetic polymers, I have included a new section providing a rough overview of this method.

As a valuable addition to magnetic resonance tomography (Section 14.4), which in the meantime has become a permanent part of medical diagnostics, a combined use of tomography and spectroscopy has developed in recent years – *Magnetic Resonance Spectroscopy*. Thus, I have described the basics of this method in a new section (14.4.2.2) and illustrated the potential of such investigations using an example from clinical practice.

I would like to express my gratitude to all those who helped me in preparing this new edition. In particular I would like to thank Professor J. Blümel, who critically reviewed the section on solid state NMR (13.2.4), Dr. R. Rensch for his untiring help in solving daily computer problems, as well as Dr. Raimund Kleiser, who supported me in writing the section on magnetic resonance spectroscopy (14.4.2.2). It is to him, as well as Dr. Hans-Jörg Wittsack of the Institute of Diagnostic Radiology, Heinrich Heine University of Düsseldorf, that I am indebted for the example shown in Figure 14-20.

In addition, I wish to thank J. Beconsall for his expert translation as well as the staff at Wiley-VCH in Weinheim, above all Dr. E. Wille, Dr. B. Bems and H. J. Schmitt, who once again was responsible for the production of this book.

Heidelberg, August 2004

Horst Friebolin