NMR: The Toolkit

Preface

The words ‘bewildering’ and ‘baffling’ are frequently found in reviews of books on nuclear magnetic resonance (NMR). They usually refer not to the texts themselves but to the vast, perplexing and ever-expanding array of techniques, applications, pulse sequences, jargon and, of course, acronyms that characterize modern NMR spectroscopy. To understand and use NMR these days, it is no longer sufficient to be adept at interpreting chemical shifts, spin–spin couplings and multiplet patterns. One must be comfortable in two, three or four frequency dimensions, relaxed about experiments on heteronuclear spin systems, excited by multiple quantum coherence and in tune with sequences of radiofrequency pulses that resemble the sheet music of a Beethoven sonata. This book attempts to explain how some of these experiments work.

Preamble

Not another NMR book? Well, yes and no. There are many excellent NMR texts on the market written for everyone from the neophyte to the connoisseur; we hope this one will be a bit different. It is intended as a short, approachable description of how modern NMR experiments work, aimed principally at those who use, or might use, an NMR spectrometer and are curious about why the spectra look the way they do. We say little about how to perform the experiments, nor do we discuss applications, both of which are well documented elsewhere. What we hope to do is to provide, in an accessible and relatively informal way, the conceptual and theoretical tools needed to understand the inner workings of some of the more important multi-pulse, multi-nuclear, multi-dimensional techniques that chemists and biochemists use to probe the structures and dynamics of molecules in liquids. There is no attempt at a comprehensive coverage.

In a sense this is two books in one, going over similar ground in different ways. In principle, one could read either independently of the other, although it would probably be wiser to begin with Chapter 1. Part A (Chapters 1–6) starts with the *vector model*, a pictorial description of simple NMR experiments, and proceeds to the more powerful *product operator formalism* with which one can appreciate the mechanics of many complex pulse sequences and predict the kinds of spectra they produce. After discussing some quite sophisticated experiments towards the end of Part A, we go back to basics in Part B (Chapters 7–10) and show how straightforward *quantum mechanics* can be used to understand NMR at a more fundamental level. Among other things, Part B attempts to show what product operators really are and to provide justifications for some of the ideas and results the reader was asked to take on trust in Part A. It will also show how one can handle experiments that are beyond the scope of product operators.

We assume the reader is broadly familiar with the fundamental interactions that control the appearance of simple liquid-state NMR spectra, namely chemical shifts and spin–spin couplings. Chapters 1–3 of P. J. Hore’s Oxford Chemistry Primer on NMR may provide a useful background; a quick glance through the parts of Chapter 6 that introduce the vector model and two-dimensional NMR might also be helpful.

Although the treatment is of necessity mathematical, we have tried to keep things as simple as is consistent with a reasonable level of accuracy. The margins carry brief reminders of bits and pieces of algebra, which the more mathematically sophisticated will probably wish to ignore. There are also a few appendices containing material that would disrupt the flow of the text; these can usually be omitted on a first reading or ignored altogether.