Preface

The American Chemical Society (ACS) recognized the Varian A-60, among the first commercial Nuclear Magnetic Resonance (NMR) instruments for use in research, which was sold in the 1960s, as a U.S. National Historical Chemical Landmark.[1] Such applications of NMR were built on the foundational discovery and knowledge of many scientists who have also earned the Nobel Prize. In the decades since those seminal developments, NMR technology has provided immeasurable advantages for society, most saliently, as a diagnostic tool in the medical setting. It has also been critical as an analytical tool for chemists, providing an expedient and relatively straightforward means for determining molecular structure while preserving the sample. Specifically, for organic chemists, the interpretation of ^{1}H NMR multiplets is among the most useful techniques for determining the molecular structure and likely identity of numerous organic compounds.

More specifically, research chemists who intend to publish an ^{1}H NMR spectrum or characterize an organic compound are tasked with accurately and reliably reporting the H–H coupling constants to support their findings. However, the complexity of some ^{1}H multiplets often discourages the investment of time needed to fully document them. This may lead to either incorrect identification or gross simplification of ^{1}H NMR spectra descriptions, where numerous NMR signals are just described as a *multiplet* (**m**). When coupling constants are not extracted, useful structural information is lost. During the undergraduate and graduate years, ^{1}H NMR spectra interpretation can seem especially intimidating due to paucity of experience and practice. For example, it is not always intuitively clear how the complex *J*-tree diagrams can be built and what the values of the true coupling constants[2] should be. In these instances, elegant practical methods and intuitive mnemonics can aid the student and researcher to develop experience and to build confidence. Equipped with this approach, and incorporating my own knowledge and experience as a Ph.D. student, postdoctoral researcher, and as a teaching assistant and an individual tutor, I have effectively made this technique and skill become an integral part of my analytical toolkit. However, it took over a decade of study, practice, and experience to arrive at that point. While many excellent textbooks exist on the subject matter, there appears to be a general trend focusing on either basic examples or covering complex, rare, and even seemingly obscure ^{1}H NMR multiplet cases. Still other textbooks focus on the math and physics that undergird the technique, which, though essential, is not particularly accessible or useful for the organic chemist in their day-to-day research.

1 Accessed June 15, 2019 at https://www.acs.org/content/acs/en/education/whatischemistry/landmarks/mri.html

2 In this workbook we refer to the coupling constants that have physical meaning as "true" coupling constants. In the literature other terms may appear: "actual" or "real." The constants that are linear combinations of the true constants may be called "apparent," "not true," or "nonrelevant."

https://doi.org/10.1515/9783110608403-201

This workbook strives to fill that apparent gap in practice, by providing a focused, step-by-step, "walk-through" of ^{1}H NMR spectra interpretation. Moreover, it heavily capitalizes on our inherent nature as visual beings and visual learners, assembling the text around copious illustration, visualization, and infographic depictions. The book strives to be a practical visual guide (and can also be thought of as a "portable tutor") that is tailored for organic chemists. It aids the reader in the interpretation of the ^{1}H NMR signals: extraction of useful constants and properly naming the multiplets. It includes carefully sequenced, guided, practice problems and visually rich answer keys to help the reader develop familiarity and experience. It also presents salient trends and provides an overall conceptual framework for the reader to organize their understanding. Notably, this book is not intended to be a scientific paper nor a literature review, but is designed to be a visual pedagogical tool. Moreover, it omits discussion of NMR theory and should not be used as a comprehensive textbook that covers all aspects and nuances of NMR spectroscopy. Readers seeking to become more specialized in the subject-matter may wish to utilize this workbook in conjunction with dedicated coursework on spectroscopy. Where possible, references are made to relevant primary authority, should the reader seek a deeper understanding.

While modern advances in NMR processing software[3] have made manual ^{1}H multiplet decryption easier, mastering it is still a fundamental skill and essential for any researcher's analytic toolkit. Obtaining and reporting appropriate coupling constants remains just as useful for structure elucidation [1, 2] as choosing the appropriate pulse sequence (in two-dimensional NMR) [3, 4]. This book takes advantage of our inherent preference for visual comprehension, and will be even more useful to those who can quickly identify patterns, schemes, structures, and tendencies, by observation.

3 For example, *http://mestrelab.com/software/mnova/* (accessed June 15, 2019).