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Preface

Today NMR is a transformative, research-enabling tool in the chemical sciences, due in part to extraordinary advances over the past 10 to 20 years. This book hopes to answer a call to action to train the next generation of scientists to be able to realize the full potential of modern NMR.

In his introduction which follows, Professor Wagner describes first-hand the extraordinary potential for NMR-enabled research to answer significant and pressing scientific questions in the public interest. He further illustrates the present state of exciting, ongoing advancements of NMR technology. We urge you to consider the impact of Professor Wagner's chapter in illustrating the need for educators to more broadly reflect modern NMR applications and methods in their curricula. The desire to address this need is one of the common threads linking together the various chapters of this book. A second major theme emerges among these chapters as well. It is the use of innovative NMR laboratory experiments to achieve improved student learning in all areas of chemistry. In other words, our authors were motivated by far more than just performing NMR for its own sake, but by the need to achieve new milestones in student learning in chemistry.

Success Leads to Challenges and Opportunities

Educators incorporating further NMR training into curricula face challenges which are linked to the successes and technological advances in the ongoing development of NMR spectroscopy.

First, cost has limited the availability of research grade instrumentation to educators. No principally undergraduate institution (PUI) operates a cryogenic probe at this time, and many offer FT-NMR at proton frequencies < 90 MHz. Furthermore, NMR instruments with four independent RF channels and specialized probes, crucially needed for biomolecular NMR studies, are rarely found at PUIs. In this book biomolecular NMR is made significantly more accessible, for example, by Harris and Driscoll who describe a web resource that allows anyone to perform a full NMR analysis of ubiquitin. Fortunately one of the most important advances has been widely adopted: magnetic field gradients. Gradients are increasingly available in NMR instruments at PUIs. Their utility in achieving automated, computer-optimized shimming, in studying molecular dynamics, and in enabling powerful new experiments is difficult to understate. Maki and Loening introduce gradient diffusion methods as well as several applications. Odeh and Li give a further example of diffusion NMR in coursework.

Second, the multidisciplinary nature of modern applications of NMR spectroscopy may appear to be a barrier to fitting NMR into core curricula. Faculty across the nation are presently discussing how to integrate NMR across the chemistry curriculum. This discussion leads to many significant issues, some of which are beyond the scope of this book: major curricular changes may ultimately be needed to adapt to the broader trend of complex technological and methodological advances permeating chemistry. However, a central role of this book is to examine and contextualize NMR in the curriculum. Fisher and Fish share their case study of NMR across the curriculum. Mueller and coworkers discuss combined theoretical and experimental priorities for integrating NMR throughout a curriculum. Steinmetz and O'Leary show how they carry NMR into advanced and seminar courses, while Goldman and Dominey demonstrate that NMR can be extremely successful in exciting and teaching students in non-majors courses. The chapter by Hanson compellingly shows how the use of automated sample-handling can be invaluable in achieving pedagogical goals.

Of special significance are the discussions and case studies given by Esselman and Mencer on incorporating NMR into high school chemistry instruction. It is not yet widely known that NMR can be found in many states' educational standards. We believe this chapter should stimulate a wider and needed effort to enhance the role of NMR in high school science education.

Finally, modern NMR methods may appear too complex for achieving meaningful, hands-on student experimentation. The advancement of NMR spectroscopy has, quite candidly, been based upon extensive use of non-trivial theoretical tools. Many chapters indicate that pedagogically significant advances in NMR theory can be incorporated into curricula. Mueller and coworkers promote the need to train students in the use of the product operator method. We also applaud Zee and Howard who introduce tensors into a laboratory experiment. Moreover, Gaede shows that exchange calculations are accessible in an undergraduate setting. And Dominey, Abrams, Kanters and Goldman introduce powerful computer visualization tools to advance students' theoretical comprehension.

Experimentation for Advanced Laboratories

Whereas NMR is often widely and effectively featured in first- and second-year coursework, there has been a paucity of options for performing NMR experimentation in advanced coursework. In the symposia and discussions that led to this book, many faculty stressed that a significant issue in incorporating NMR across a curriculum is the need for more laboratory development in the latter years of an undergraduate degree. This book aims to describe a rich set of new experiments, tested and evaluated, that address this need.

In physical chemistry, Grushow and Sheats describe a suite of experiments that drive student learning in numerous areas. DeVore and coworkers give an innovative gas phase experiment with elegant thermodynamics. Maki and Loening describe the accessibility of diffusion measurements for the study of molecular transport and give a sound introduction to the topic.

Chapters by Harris, Trumbo, Zee and Howard, and Rovnyak and coworkers address the need for more options for NMR in biochemistry and biophysics. Significantly, these chapters have a theme of increasing student learning at the interface of biochemistry and structural biology.

Options for advanced organic instruction are given in chapters by Gaede, Odeh and Li, and O'Leary and Steinmetz. Where O'Leary and Steinmetz push the boundary for organic structure solving with students, Gaede and Odeh and Li join other authors in this book in developing experiments that allow students to witness and measure molecular dynamics.

Metal promoted transformations comprise a wide variety of key processes in chemical and biological systems. The use of NMR spectroscopy to probe the coordination environment and stereochemistry of the metal complexes facilitates a greater understanding of the critical reaction parameters. Despite the importance of this technique, inorganic NMR spectroscopy often receives only a cursory glance in educational settings. To address this deficiency, the chapters by Nataro, Minelli, Hawrelak, and Uffelman outline the synthesis and characterization of metal containing complexes that offer a range of unique spectral properties.

The material presented in these chapters can be incorporated into both lecture and laboratory courses in order to broaden the coverage and depth of the NMR discussion.

Permanent Magnet FT-NMR

Permanent magnet NMR spectrometers equipped with a pulsed, Fourier-Transform upgrade (Anasazi Instruments, Inc.) are widely used in chemistry education and are an area of a good deal of significant and recent pedagogical research, carefully reviewed by Abe and Contratto, who also show a new imaging experiment. Chapters by Niece and Moyna, Collins and Amel, and Goldman and Dominey all show the versatility and power of this instrumentation in achieving pedagogical goals.

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