Contents

Preface ............................................................................................................................................. xi

1. Introduction to NMR Spectroscopy in the Undergraduate Curriculum ............ 1
   Anton S. Wallner, Laura J. Anna, and David Soulsby

2. Modern NMR Experiments: Applications in the Undergraduate
   Curriculum ................................................................................................................................... 7
   David Soulsby

Organic Chemistry

3. Data versus Dogma: Introducing NMR Early in Organic Chemistry To
   Reinforce Key Concepts ............................................................................................................. 45
   Paul A. Bonvallet and Judith C. Amburgey-Peters

4. Using NMR Spectroscopy To Promote Active Learning in Undergraduate
   Organic Laboratory Courses ..................................................................................................... 57
   John A. Cramer

5. NMR Spectroscopy in Nondeuterated Solvents (No-D NMR): Applications
   in the Undergraduate Organic Laboratory .............................................................................. 69
   John E. Hanson

6. Overcoming Problems Incorporating NMR into the Organic Chemistry
   Lab .............................................................................................................................................. 83

7. Using NMR To Investigate Products of Aldol Reactions: Identifying Aldol
   Addition versus Condensation Products or Conjugate Addition Products
   from Crossed Aldol Reactions of Aromatic Aldehydes and Ketones ......................... 91
   Nanette M. Wachter

8. Use of HSQC, HMBC, and COSY in Sophomore Organic Chemistry Lab .... 103
   V. R Miller

Inorganic/Heteronuclear Chemistry

9. $^{31}$P NMR Spectroscopy in an Undergraduate Inorganic Curriculum ............ 131
   Chip Nataro, Chelsea L. Mandell, and Margaret A. Tiedemann
10. Using $^{195}$Pt and $^{31}$P NMR To Characterize Organometallic Complexes: Heteronuclear Coupling in the Presence of Geometric Isomers ..................... 155
Daron E. Janzen, Mainong Hang, and Hannah M. Kaup

11. Beyond Ordinary Undergraduate Experiences: Routine Measurements with Heteronuclear, Heterogeneous, and Paramagnetic Samples ............... 169
Patrick J. Desrochers

**Physical Chemistry and Biochemistry**

12. Substituent Interactions in Aromatic Rings: Student Exercises Using FT-NMR and Electronic Structure Calculations ........................................ 189
James B. Foresman and Donald D. Clarke

13. Using NMR Spectroscopy To Elucidate the Effect of Substituents on Keto-Enol Equilibria ............................................................................ 205
Anderson L. Marsh

14. NMR-Based Kinetic Experiments for Undergraduate Chemistry Laboratories .................................................................................................. 211
Eric J. Kantorowski, Bijan D. Ghaffari, Allee Macrorie, Kellan N. Candee, Jennifer M. Petraitis, Melanie M. Miller, Gayle Warneke, Michelle Takacs, Vanessa Hancock, and Zoe A. Lusth

15. Physical Chemistry Laboratory Projects Using NMR and DFT-B3LYP Calculations ..................................................................................... 229
A. C. Bagley, C. C. White, M. D. Mihay, and T. C. DeVore

16. $^{1}$H NMR MAS Investigations of Phase Behavior in Lipid Membranes ........ 245
Holly C. Gaede

**NMR Spectroscopy Across the Undergraduate Curriculum**

17. Vertical Integration of NMR in the Chemistry Curriculum: A Collaborative Advanced Laboratory Experiment Examining the Structure-Reactivity Relationships in Carbonyl Reduction ........................................... 261
Sheila R. Smith and Simona Marincean

18. NMR Spectroscopy in the Undergraduate Curriculum at the University of Notre Dame .................................................................................. 275
Steven M. Wietstock, Kathleen A. Peterson, DeeAnne M. Goodenough Lashua, Douglas A. Miller, and James F. Johnson
NMR Spectroscopy: Collaborative Strategies, Resources, and Grant Writing

19. Oregon NMR Consortium: A Collaboratory for NMR Data Acquisition and Processing ................................................................. 293
   R. Carlisle Chambers

   Antony J. Williams, Valery Tkachenko, and Alexey Pshenichnov

21. Writing More Competitive Grant Proposals for NMR Spectrometers: Research and Curriculum Programs of the National Science Foundation .... 321
   Thomas J. Wenzel

Editors' Biographies .......................................................................................................................... 335

Indexes

Author Index ................................................................................................................................. 339

Subject Index ............................................................................................................................... 341