

INTERPRETATION OF NMR SPECTRA

A n E m p i r i c a l A p p r o a c h

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by

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Preface

In writing this book I had two main objectives: (1) to teach the organic chemist how to interpret proton magnetic resonance spectra, and (2) to provide the reference data which are constantly needed in the use of proton spectra. I have felt that it was important to point out not only the information which can be gained from spectra, but also the limitations and the potential pitfalls. All of the important facts are organized into tabular summaries. Every effort has been made to present the material clearly, concisely, completely, and accurately. At the same time, subjects not directly related to the interpretation of spectra have been omitted. Thus, while the conclusions drawn from theory are presented, the theory itself has been avoided.

There are a number of advantages in learning the empirical facts before learning the theory. First of all, in interpreting spectra one usually has to rely on his knowledge of the accumulated empirical correlations much more than on his knowledge of the theory. In fact, one could know all of the theory and still not be able to interpret spectra unless he also knew the empirical facts. Secondly, the theory is much more easily understood after the facts have been mastered.

This book began as a seminar for my colleagues at G. D. Searle & Co. The objective of that seminar was to present all of the fundamentals needed in the interpretation of proton spectra. That material, which constitutes Chapter 2 of this book, was later assembled as a booklet for use in conjunction with a workshop presented at Searle by Dr. Harmon W. Brown, Jr., and Dr. Donald P. Hollis of Varian Associates.

My functions in writing this book have been primarily to collect, evaluate, organize, and present the material in terms familiar to the organic chemist. I have drawn heavily from the texts by L. M. Jackman; J. A. Pople, W. G. Schneider, and H. J. Bernstein; K. B. Wilberg, and B. J. Nist; and J. D. Roberts. In addition, I gained much information from the series of lectures at Searle by Dr.

Harmon W. Brown, Jr., and Dr. Donald P. Hollis of Varian Associates, and from lectures elsewhere by Dr. Frank A. L. Anet, Dr. Kenneth W. Bartz, Dr. Wallace S. Brey, Jr., LeRoy F. Johnson, Dr. Paul C. Lauterbur, Dr. John A. Pople, Dr. John D. Roberts, Dr. James N. Shoolery, and Dr. George Slomp.

A number of points were clarified in discussions with Dr. Fred Kaplan, Dr. Thomas J. Flautt, and Dr. Frank A. L. Anet.

My colleagues at Searle have contributed to this book in many ways. They have brought much literature to my attention, pointed out many unusual features in spectra of their own compounds, and have challenged me with many questions.

The unique research environment at Searle has been important both in my own study of NMR and in the development of this book. I am particularly indebted to my supervisors, Dr. Robert R. Burtner, Dr. Byron Riegel, and Dr. Albert L. Raymond, for their support in this project.

Most of the spectra used were determined by Miss Diana Ede under the direction of Aristides J. Damascus, supervisor of the spectral laboratory at Searle. The spectral laboratory is part of the Analytical Department, which is administered by Dr. Robert T. Dillon. The enthusiasm, ability, and support of this group has been essential to this book.

The graphical treatment of the ABX system given in Chapter 4 was worked out in collaboration with David W. Calhoun, who served as my principal consultant in mathematics.

I am especially indebted to my wife, Harriett, and to Edward A. Brown and Dr. Thomas J. Flautt for their careful reading of the manuscript. Their criticisms have led to considerable improvements in all aspects of this text.

In addition to being my chief critic, my wife also shouldered many responsibilities which permitted my completion of this book in a reasonable length of time.

I am grateful to Dr. Kenneth B. Wiberg, Dr. Bernard J. Nist, and W. A. Benjamin, Inc., for permission to reproduce the material given in Figure 4-4, and to Varian Associates for permission to reproduce a number of spectra.

The original draft of Chapter 2 was typed by Mrs. Karen Khubchandani. The present manuscript was typed by Mrs. Diane George and Mrs. Sandra Blume. Many of the structures were drawn by Mrs. Blume, who did much of the art work in the original draft of Chapter 2. I have also been aided during the development of this

book by the photographic work of Clifford Kornoelje and the multilith work of George Wolfram and Phillip Sosnowski.

The efficient and pleasant staff of Plenum Press did much to improve the presentation of the material.

Criticisms of this book will be appreciated. In particular, comments concerning residual errors or the emphasis placed on specific topics will be helpful in the preparation of possible future editions.

Roy H. Bible, Jr.

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