CRC

Atlas *of* Spectral Data *and* Physical Constants *for* Organic Compounds

Jeanette G. Grasselli

CRC PRESS

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published by

A Division of THE CHEMICAL RUBBER CO., 18901 Cranwood Parkway · Cleveland, Ohio 44128

International Standard Book Number 0-87819-032-5
Library of Congress Card Number 72-94345

Printed in the U.S.A. by Rand McNally & Company

PUBLISHER'S PREFACE

The publication of the CRC Atlas of Spectral Data and Physical Constants for Organic Compounds represents the culmination of more than two years of dedicated effort by Mrs. Jeanette Grasselli and her associates. Looking only at the physical proportions of the work, it is a staggering production. Comprising almost 1800 oversized pages, it contains well over one million pieces of evaluated data. The expertise required to organize and produce the Atlas is tremendously impressive. The courage to undertake and complete the task is awe-inspiring.

Although the Atlas is a giant step forward, it is, nevertheless, only the first step of an immense design. The concept emerged five years ago when it became apparent that the vast quantity of scientific data could be managed only by the employment of innovative techniques and new technologies.

The ultimate plan conceived at that time was to create a computerized databank with virtually unlimited capability for storage and retrieval. Even more important, however, would be the organization of programs to provide for instantaneous output in almost any useful format. Utilizing a centralized computer installation, a microwave transmission system, and thousands of terminals in strategic locations, a simple keyboard would unlock a storehouse of scientific information.

The broad concept was clear and compelling, its conversion to reality a forbidding conglomeration of unsolved problems. After almost three years of searching and researching, dreaming and scheming, conferences, surveys, and field trips, one major premise was established beyond any reasonable doubt: the complete program as originally visualized could not be brought into being at a single step, at a single time, as a single package.

The difficulties to be overcome included aspects of computer technology, economics, and education. Above all, however, was the problem of building a database large enough to justify the system. Computerized banks of literature citations, indexes, and even abstracts were common enough, but a viable base of "hard" data, broad enough in magnitude and potential application, was nonexistent.

At this point, it was clear at last that the only promising approach to the ultimate goal was a patient, plodding effort to produce a database of far-reaching scope and content. The selection of organic compounds for the subject was a natural and logical choice due to the type and quantity of data available, and, even more important, the usefulness and, therefore, the probable demand and acceptance by the scientific community.

Now the task was established and the work could begin. It was determined that the first segment would consist of the compilation and evaluation of the spectral data and physical properties for approximately eight thousand organic compounds presented in printed format. This project has now been completed and the First Edition of the CRC Atlas is an accomplished fact.

The significance of the achievement is highlighted not only by its inherent value as a reference tool but also as a confirmation of the feasibility of the program. This significance is in no way diminished by frank recognition of the formidable effort which still lies ahead. In truth, the dynamic character of this type of scientific information precludes the possibility of ever completing the task.

Viewed in perspective, however, a beginning has been made which is of real substance and even greater promise. We congratulate Mrs. Grasselli and her associates. As publishers, we enjoy a deep sense of pride and satisfaction in presenting the First Edition of the Atlas. We offer it as concrete and tangible evidence of our optimism, and of our dedication to a vision of great purpose, of boundless proportions and of infinite potential.

B. J. Starkoff, President
THE CHEMICAL RUBBER Co.

The concept for the publication of an Atlas of Spectral Data and Physical Constants for Organic Compounds was first described to me by B. J. Starkoff, President of The Chemical Rubber Co., some two years ago. His enthusiasm was dynamic and contagious, his vision bold and intriguing. I was captivated by the potential usefulness of the work as a unique reference aid.

For the first time, comprehensive data including the name, synonyms, empirical and structural formulas, Chemical Abstract Registry No., Wiswesser Line Notation, boiling point, melting point, density, refractive index, specific rotation, solubilities, molecular weight, literature references, and infrared, ultraviolet, nuclear magnetic resonance and mass spectral data were all to be combined in a single volume for desktop use. The production of the Atlas has been an exciting, always challenging, often frustrating endeavor.

The first decision concerned the mode of presentation of the spectral information. The basic objective was to compile accurate data of uniform high quality and to present it in a useful format. It was desired to keep the material concise and display it along with the other physical constants on each compound in the *Master Data Table, Table 1, Section B.* Careful coding criteria were established, the most reliable spectral reference catalogs were utilized, and a very sincere effort was made to evaluate the data as they were coded. The specific procedures used to meet these objectives are described in the *Explanation to the Table, Section B.* It is worth noting, however, that the spectral data were coded with emphasis on selecting values characteristic of compound structure, not necessarily striving for a complete representation of the original spectrum.

The physical constants given for each compound are those judged to be the most meaningful, and are abridged from the Tables of Physical Constants of Organic Compounds, CRC Handbook of Chemistry and Physics. A critical review and upgrading of these is planned for each edition of this Atlas so that the data base remains viable and, above all, useful.

The inclusion of Wiswesser Line Notation for each compound is an innovation, but for those willing to expend a small effort to become familiar with its concise and unambiguous representation of chemical structure, it should prove to be a powerful aid in compound searching and identification. For this reason all of the indexes to spectral data in the Atlas incorporate an "Eyeball" feature, based on WLN, which greatly enhances the value of the index. A description of WLN and "Eyeball" is given in Section C, Part II.

The Atlas can be used to obtain information, including spectral data, on approximately 8000 compounds, or conversely, to identify an unknown from some characteristic physical constant or from spectral data. A set of comprehensive indexes is given in Section C. Their application is explained in the foreword to each. Some of the spectral indexes are entirely new in their organization of the data. This is a calculated experiment and I earnestly solicit the advice and criticism of users of the Atlas on their effectiveness. We hope to continually expand and improve these indexes in subsequent editions.

The spectra-structure correlation charts in Section A should be helpful in the identification of unknowns. They are basic to the use of spectroscopic methods. The remainder of Section A contains ancillary spectroscopic aids and general information of interest to those engaged in obtaining or interpreting spectral data.

Successful utilization of this Atlas depends upon recognition of the basic philosophy inherent in its organization and content. It is widely accepted that spectral data are of immense value in solving analytical problems, or in determining identity or structure of unknown materials. The enhanced status of spectroscopic methods should not contribute to a disregard for the importance of other physical constants of a substance. Certainly the most rapid route to unambiguous identification of materials is to bring several pieces of information to bear on an unknown. The Atlas provides a basic reference collection of physical constants and spectral data on organic compounds to facilitate such identifications. This work is dedicated to that aim.

We well recognize that with the massive amount of data handled to assemble this Atlas, errors or omissions are likely to be found. Corrections, criticism, and suggestions for improvement from users of the Atlas will be very welcome. For this purpose a convenient, pre-addressed stamped tear-out form has been included as the last page of the Atlas. We are already replete with ideas for the second edition, and we eagerly await your comment.

The Atlas could not have been completed without the conscientious and careful work of the coding teams working under the guidance of the members of the Advisory Board. They are individually listed as contributors and I wish to express my thanks to them all. The brilliant programming of T. L. O'Connor of Chi Corporation produced an organized and beautifully executed book (see special note from Chi Corporation) from what appeared to be a bewildering array of unrelated coding forms and keypunch cards. His patience and keen intelligence made my task immeasurably easier. The editorial staff at Chemical Rubber Co., especially Earl Starkoff, Gerald Becker, Florence Thomas, and Kay Harter, were indispensable in providing encouragement, advice and instruction into the new, for me, world of a successful publishing house. Their attention to detail and careful assembly of the material from this truly unique printing method deserve recognition. Finally, I would like to gratefully acknowledge the official and undiminished support of my superiors and my associates at The Standard Oil Co. They made every harried day and deadline easier to bear by their patient understanding and unfailing help, and I most sincerely thank every one of them.

Jeanette G. Grasselli

SPECIAL NOTE BY CHI CORPORATION

Computers, Chemistry and Photocomposition:
The Production of the Atlas

Computers affect virtually every aspect of our lives today. They are programmed to do everything from calculating the interest on your savings account to keeping the shelves of your local supermarket fully stocked; from designing bridges to flying men to the moon and back. With the exception of the moon flight, all of these tasks are physically possible without the computer. But the complexity of these jobs, not to mention the sheer volume of computation involved, makes it impractical to consider them apart from the computer.

The Atlas of Spectral Data falls into this class also. Although this book could have been manually composed using conventional techniques (as it would have been ten years ago), those of us responsible for its production shudder at the very thought. The difficulty of assembling data for the various tables and then proofreading for accuracy would have forced publication years into the future, and increased its cost many times.

The role of the computer (Chi Corporation's Univac 1108) has been threefold. First, it was programmed to store and maintain CRC's complex and extensive data base (15,000 compounds, and growing, as of this writing). Second, it was programmed to extract from the data base the information needed for the various tables and sort it into an order useful for each index (e.g., ascending by boiling point and descending by Chemical Shift in the NMR). Third, it was programmed to control a sophisticated high speed phototypesetter (the Harris Intertype Fototronic CRT) to produce camera-ready masters for 22 of the tables and indexes found in this book. Certainly one of the most interesting aspects of this project is that the finished product handed to the printer was almost entirely machine produced – and at a rate of three to four pages per minute!

It was a challenging undertaking. Each step presented us with problems, as well as the satisfaction of seeing a difficult job properly done. During the first phase, as Mrs. Grasselli and her staff encoded data for the Atlas, we all rediscovered the First Axiom of Computing: Garbage In, Garbage Out. During the second and third phases, the format and structure of some indexes changed almost daily as we discovered unexpected patterns in the data. But these frustrations were generally forgotten as we invented useful ways of presenting our findings to the reader. For example, the addition of subscripted multipliers to the EYEBALL column is the proud innovation of this author and Dr. Norman Pollack. In short, it was a massive effort, but the results have made it worthwhile.

T. L. O'Connor, G.F.W.

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