# NEW BOOKS

edited by F. W. Quackenbush

Acetylenic Compounds: Preparation and Substitution Reactions, by Thomas F. Rutledge (Reinhold Book Corporation, New York, 342 p., 1968, $20.00).

The book contains eight chapters, three of which are subdivided into six parts each; each chapter or chapter part has its own index.

As the first of two planned, this book discusses the preparation, substitution reactions and some uses of acetylenic compounds (while the second, to be published in 1969, will cover preparation of allenic compounds and the addition reactions of acetylenes and allenes). The first three chapters deal with structure and properties, experimental aids for handling, purification and analysis, and preparation by elimination reactions. The fourth chapter treats substitution of acetylenic hydrogen by other elements (six parts); the fifth, ethynylation and alkynylation (using stoichiometric amounts of base, by alkali metal acetylides, by Grignard reagents, by catalytic reactions, of dicarbonyl compounds, by the Mannich reaction); the sixth, coupling reactions. The seventh chapter treats cyclic and macrocyclic acetylenes (small ring acetylenes and allenes, macrocyclic non-conjugated, conjugated macrocyclic polyacetylenes containing amomatic rings, macrocyclic polyacetylenes containing oxygen or sulfur atoms, conformation of cycloalkynes and other flexible macrocycles); the eighth chapter, acetylenic compounds as drugs.

Since the publication of R. A. Raphael's "Acetylenic Compounds in Organic Synthesis" in 1955, there has been a very large and expanding interest in this field. Dr. Rutledge attempts to cover both the old and recent chemistry effectively, if not encyclopedically, within moderate space. In this he has been highly successful. Many significant new developments are described. He furnishes enough details of the most important reactions to provide readers with a good background and with leads into the pertinent literature. The frequent indication of reaction mechanisms is a valuable feature of the book. The coverage of recent literature appears to be very good: one page of 41 references afforded 21 published in 1960–64, 7 in 1965, 5 in 1966 and 1 in 1967.

In the timely exposition of many facts in little space the author has consciously sacrificed something of literary style; the reviewer did not find this objectionable. Formulas are misprinted, however, on pages 33 and 50. On page 323 in a pregnenynone formula, a 19-nor carbon is shown and a 5(10) double-bond omitted. There are several minor printing errors.

This book should be on the bookshelf of every research chemist concerned with the subject. It would also be useful as an adjunct to a related academic course.

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Newer Methods of Preparative Organic Chemistry, Vol. 4, Edited by Wilhelm Foerst (Verlag Chemie GmbH, Weinheim/Bergstr., Academic Press, New York, 348 p., 1968, $15.00).

The most recent edition of this useful series concerned with preparative organic chemistry contains seven sections, six of which are in keeping with the format of the series. The seventh section, by far the longest, is a complete review of the use of complex borohydrides and of diborine in organic chemistry. Although this chapter is not consistent with the earlier chapters, it is a most useful and comprehensive review of borohydride chemistry, complete with 1900 references.

Although the context of the book is taken from reviews which appeared in Angewandtc Chemie, the articles have been brought up-to-date and the authors are all well-qualified for such a presentation. The first chapter, Alpha Additions to Isonitriles—Triple Additions and Four Component Condensations, is a detailed review of the Ugi reaction, including a discussion of the Passerini reaction. The second chapter, concerned with isonitrile syntheses, is quite complete and includes a host of tables and reaction procedures which the laboratory worker will find most useful. The third chapter is concerned with the reactions of sodium hydrazide with organic compounds. The chapter is sub-divided into addition reactions, substitution reactions, reduction reactions, cleavage reactions and dehydrogenative hydrazination of dienes. The free radical mechanism and procedure terminate the chapter. The fourth chapter concerned with ethynation reactions is a comprehensive review of the reactions of alkynes with various organic substrates. The remaining two chapters are concerned with the syntheses with nascent quinones and cyclization of dialdehydes with nitromethane. Again, both chapters are quite comprehensive and complete. As stated earlier, the balance of the volume is comprised of a comprehensive review of complex borohydride chemistry.

In general, the format is excellent and each chapter is well documented with references, reaction mechanisms and excellent drawings. Much of the data is presented in tabular form, and, in all cases, reaction mechanisms are clearly depicted and explained. The book is quite up-to-date. The chapters are complemented by a fairly complete bibliography. The subject index is extensive, although the writer feels that it could have been expanded somewhat more since there are so many specific compounds mentioned in the volume. In many instances, actual laboratory procedures are described in detail, and in some cases, recommended apparatus is depicted. In general, the translation is excellent, and one feels the original articles were written in English. There are very few typographical errors in the book, the most prominent of which is the wrong Library of Congress card number.

In summary, this volume, with the exception of the last chapter, is in keeping with the format of previous volumes and fulfills a very useful function. The book is to be recommended for every chemical library and for purchase by most graduate students in organic chemistry and academic organic researchers. It will be an invaluable aid to industrial workers involved in the specific or related areas of research. This type of series of reviews has a very important place in our advancing field of organic chemistry, and it is hoped that the series will be continued.

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A New Chemical Structure Code for Data Storage and Retrieval in Molecular Spectroscopy by L. C. Thomas (Heyden & Son, Ltd., Spectrum House, Alderton Crescent, London, N.W. 4, England, 60 p. 1968, $4.00).

The format of this little publication resembles more an individual number of a current technical journal than that of a reference text. The principal objective of the text is to describe an optical coincidence system for infrared spectral retrieval, known as the Kodak Miracode System. Miracode is an abbreviation for Microfilm Information Retrieval Access Code. The Miracode System is not new, having been used for library retrieval for several years. Its use in connection with an infrared absorption spectra retrieval program was described in this country by Jonkers Business Machines, Inc., several years ago.

Two quotations from the introduction to the book express the need for an infrared spectral retrieval system and the need for a large number of reference spectra as part of any such system:

"The identification of a chemical compound by means of its infrared spectrum depends on the comparison of the spectrum with that of an authentic sample of the compound, and confirmation that the two spectra are identical. The efficiency with which identification can be carried out therefore depends on the ready availability of adequate reference spectra."

"Molecular structure determinations by infrared spectroscopy, therefore, depend on the ready availability of a large number of reference spectra and on the ability to retrieve an individual spectrum from the collection by name, by empirical formula, by structural groups or by band positions."

Systems of spectroscopic data storage are first considered, starting with the most obvious, and probably the least satisfactory, merely filing spectra in numerical order. An improvement on this system is an alphabetical file based on the names of the compounds which permits some presorting. Additional entries can be filed in their proper places and similar compounds can be arranged together, for example all organophosphorous compounds can be grouped in one separate file. The third filing system considered is microfilm filing, obviously the most compact method of storing spectroscopic data.

Various systems of retrieval are considered starting with mere mention of the simplest systems based on a numerical or alphabetical file. The first system based on coded spectra is the Sadtler Spec Finder, which is described in detail, but considered impracticable for anything but the smaller collection of spectra. Punched card systems are next considered, including the edge-punched hand sorted cards illustrated with a description of the DMS (Documentation of Molecular Spectroscopy) system, and machine-sorted overall punched cards of the Wyandotte-IBM card in the ASTM (American Society for Testing and Materials) System. Curiously, computer retrieval receives only scant attention.

The hand sorting of numerical or alphabetical files, the Spec Finder, or of the hand sorted edge-punched or machine sorted overall punched cards are all considered to become inadequate as the number of spectra to be retrieved increases. The computer system, on the other hand, is considered impractical for general use. The very brief description of computer searching and retrieval is introduced with the words "In theory, the library of spectroscopic data could be stored in, and searched by, a computer." This appears to be a somewhat over conservative statement to appear in October 1967, when such systems were in daily use in scores, probably hundreds of spectroscopic laboratories. The conclusion regarding the potential use of computers for spectroscopic retrieval is equally puzzling, "Although the ability of the computer to do all this, and more, is beyond question, this is still hardly the solution to the spectroscopists' data storage and retrieval problem."

The Kodak Miracode system is described in detail and its adaptation to spectroscopic data retrieval is then discussed. Use of the system for infrared absorption data is illustrated for nine compounds. From page 18 through 35, coded data are tabulated on even-numbered pages and the corresponding spectra reproduced on the odd-numbered pages. The booklet contains a 21-page appendix listing the Chemical Structure Code. To this reviewer, the limitations cited for the use of all retrieval systems described (other than the use of computers) applies to the Miracode. The system does not meet the requirements of the author, who established in his introduction that it depends upon "the ready availability of a large number of reference spectra." Only 500 spectra can be placed on a single reel of film and permit space for other data essential for retrieval. Thus, 200 reels would already be required to handle the 100,000 spectra now available through the ASTM program. The book does, however, provide a very adequate description of the interesting optical coincidence system, the Kodak Miracode System with several applications of its use in the special problem of retrieval of infrared absorption spectra.

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Modern Methods of Chemical Analysis by Robert L. Pecsok and L. Donald Shields (John Wiley and Sons, Inc., 480 p., 1968, $9.95).

This introductory text represents a significant departure from the familiar textbook on quantitative analysis. Traditionally included subjects such as gravimetric and volumetric analysis have been replaced by such topics as separations, spectrophotometry, electrochemistry and radiochemistry. Applications are emphasized in the field of organic chemistry as well as biochemistry. The depth of coverage is substantial. References are frequently given to selected sources to supplement the text. The book is recommended as an introduction to instrumental methods of analysis and would be useful to technicians and others who desire a survey of new techniques.

The book is divided into topics by chapters. Chapters 2 through 7 concern separation techniques starting from simple phase changes and going through various kinds of chromatography. Chapters 8 through 13 treat the nature of electromagnetic radiation and its interaction with matter including qualitative and quantitative spectrophotometry, nuclear magnetic resonance and mass spectrometry. Chapters 14 through 17 cover the more classical topics of electrochemistry and acid-base chemistry in aqueous and non-aqueous solvents. Finally, Chapters 18 through 19 introduce kinetics as applied to rates of reactions and radioactivity.

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NMR Band Handbook by Herman A. Szymanski and Robert E. Yelin (IFI/Plenum, New York, xiv + 432 p., 1968, $12.50).

The reader familiar with Dr. Szymanski's "Infrared Band Handbook" and its four supplements (See Reviews JAOCS *41,* 32, 1964; *43,* 73A, 1966; and *45,* 528A, 1968) will readily recognize the format of this text. Each page contains 12 box-shaped tables of NMR data; pages 1 through 399 account for 4777 such tables. These compilations are restricted to proton magnetic resonance. Each table represents a proton in a specific molecular environment, that is, a proton exhibiting a different chemical shift. We are told, in the introduction, that the approximately 4800 proton chemical shifts, thus represented, are collected from some 1200 compounds.

Data are entered into the Handbook according to proton code designations. The method of coding protons is described in detail in section II of the introduction with several examples including special provisions for coding olefinic and phenyl protons. Proton chemical environments are classified into 1 of 21 main functional groups, containing the proton and designated by Arabic numerals 1 to 21. Groups alpha or beta to the proton being coded (or ortho in the case of phenyl protons) are classified as subgroups or as sub-subgroups, respectively, and designated with capital letters and lowercase letters, respectively. Once the rather simple task of mastering the proton code designation system is accomplished, location of the chemical shift for a specific type of proton should be readily achieved. To assist in the location of a specific proton the tabulation of structural groups to which the code numbers and letters are assigned, as given in the introduction, is repeated in a foldout which can be placed in just position with any page of the text. The entire alpha numerical code that is used in the presentation has been borrowed intact from the NMR Spectra Catalog of Varian Associates. It is, therefore, probably familiar to many NMR spectroscopists. Others, who are not acquainted with this code, may want to refer to the NMR Spectra Catalog of Varian, particularly for many additional examples of its use.

Each of the 4777 tables which comprise the Handbook contain, therefore, data relevant to a proton in a specific molecular environment, as measured from the spectra of some 1200 molecules. The structural formula occupies the center of each table, with each proton with a different chemical shift designated with a lower-case letter in parenthesis. These designations have no relation to the proton code designation, but rather refer to the chemical shift data. In the upper left hand corner of each table the proton code designation is given. The upper right-hand corner of each table is reserved for the spectral shift data, presented in three columns; the lowercase letter which indicates which of the protons from the structural formula of the molecule is being measured; the chemical shift; and a peak designation. This peak code designation has been devised to give the reader at least some qualitative visualization of the proton line pattern. The designation in the upper right-hand corner of each table refers to a peak code table of 42 proton peak patterns, given in the introduction and again, for convenience, repeated in the foldout. The proton used to establish the proton code designation for the entry in the table in question is indicated by an arrowhead.

The molecular formula is found in the lower left-hand corner of each table, followed in the center of the lower line by the name of the solvent and the concentration of the sample. The lower right-hand corner contains a designation from which the source of the NMR spectra can be obtained. In addition to the proton code designation arrangement of the data, the Handbook is augmented by an "Index of Molecular Formulas" and by a "Shift Index."

Unlike infrared absorption bands, where the number of observed fundamental bands is complicated by the patterns of overtone, combination and difference bands, making fingerprint comparisons an almost necessity complement to group-frequency correlations and requiring that any collections, to be at all adequate, must number in the order of tens of thousands of specific spectra, the NMR spectra of approximately 4800 different protons, or otherwise stated, of chemical shift data of the proton in some 4800 different molecular environments, would appear to be a considerable assistance to a research worker attempting to confirm a hypothetical structure or to hypothesize an alternate structure.

The quantity of data that Drs. Szymanski and Yelin have made very readily available would appear to make the Handbook indispensable to the worker in this specific field. It is difficult to understand why any NMR spectroscopists engaged in these types of problems would want, or indeed could afford, to be without it.

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CHEMISTRY, PHYSICS AND APPLICATION OF SURFACE-ACTIVE SUBSTANCES, Vol. 1, Chemistry of Surface-Active Substances, by F. Asinger. One of three volumes on the Proceedings of the IVth International Congress on Surface-Active Substances. Brussels, September 7–12, 1964. (Gordon and Breach Science Publishers, lx + 549 p., 1967, $39.00.)

For the first 60 pages the book is quite confusing with the sections on Preface, Committee Membership, Welcome, Allocution, Opening Address, Conference Thoughts, Congress Opening and Closing Addresses, another Preface, Foreword and Table of Contents (for Vol. 1, 2 and 3) in either French, German or English. Some portions are given in multiple language while others are not—hence the confusion.

The major sections of the Congress as compiled in

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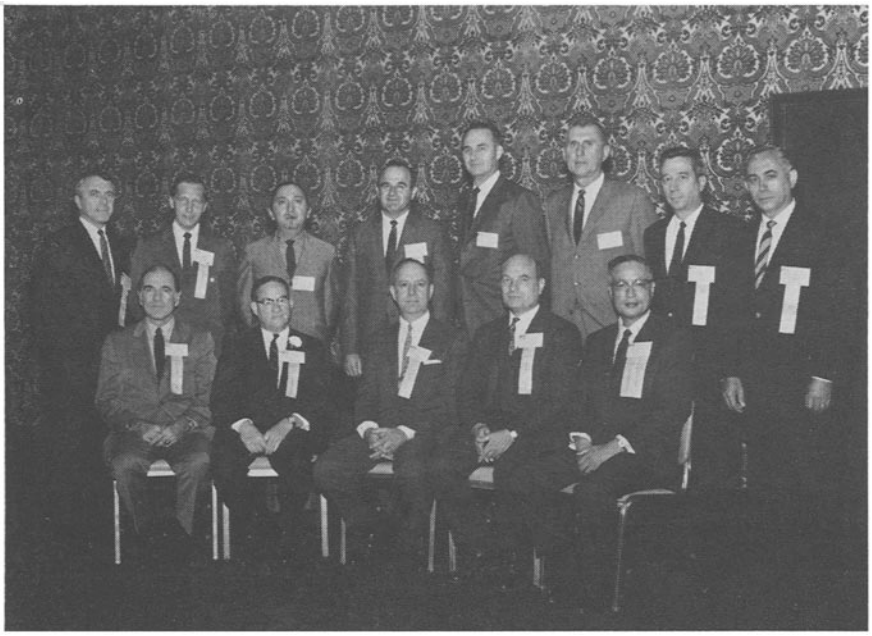
# Host Committee '68 Fall Meeting

It has come to our attention that a group picture of the Host Committee for the 1968 Fall Meeting did not appear with the pictorial review, so we present them now.

Left to Right, Standing: A. M. Rossetto, Jr., Co-Chairman, Registration and Printing Comm.; J. J. Geminder, Chairman, Hotel Comm.; Manuchehr Eijadi, Co-Chairman, Entertainment Comm.; Frank Naughton, Chairman, Registration and Printing Comm.; D. J. Meshnick, Co-Chairman, Publicity Comm.; E. P. Horvath, Co-Chairman, Finance Comm.; J. P. McNaught, Co-Chairman, Hotel Comm.; J. F. Anodide, Chairman, Finance Committee. Left to Right, Seated: H. G. Salomon, Chairman, Fund Raising Comm.; E. I. Marshack, Chairman, Entertainment Comm.; F. B. White, General Chairman, E. A. Lawrence, General Co-Chairman, S. S. Chang, Chairman, Program Committee. Not shown: Mrs. E. A. Lawrence, Chairman, Ladies Comm.; Mrs. Peter Kalustian, Co-Chairman, Ladies Comm.; Mr. Robert Casparian, Chairman, Publicity Committee.



**42nd Fall Meeting General Chairman F. B. White (front row center) poses with his 1968 New York Committee Chairmen.**

## • New Books....

(Continued from page 151A)

this book are: Terminology, Constitution and Properties, Synthesis and Manufacture, Analytical Methods and Subject and Author Index. Of the 48 papers presented, 24 are in English while the rest are in French or German and will require translation for the average reader.

The original papers themselves are worthwhile and represent respectable pieces of work on the various topics covered. Each article is summarized at the beginning of the article a bit too briefly for this reviewer's taste, in the three languages, regardless of whether the complete article is in French, German or English. References at the end are most helpful.

Analytical techniques and problems discussed in the last section appear to be particularly worthwhile and pertinent.

In general, this volume represents papers presented in 1964 and would be most useful as a reference type of work for libraries, large corporations and for individuals who are highly specialized in various areas of surfactant chemistry.

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Qualitative Organic Chemical Analysis by W. J. Criddle and G. P. Ellis (New York Plenum Press, 119 p., 1967, $6.00).

The aim of this text is primarily to introduce an approach to the identification of organic compounds by chemical identification of functional group(s) present. The author intended his simplified text to be supplemented by lectures on the theoretical basis of the various chemical tests. Pages 1 through 46 describe preliminary and functional group tests, the separation of organic mixtures, and the preparation of derivatives. Pages 46 through 115 present tables which principally provide melting and boiling point data useful in characterizing organic compounds and their derivatives. No references to other sources are given. The text would be useful as an abbreviated introduction to qualitative organic chemistry or as a quick reference to qualitative or organic tests.

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## Long-Time AOCS Member Dies

K. T. Holley, ('45) Chemist Emeritus of the Georgia Experiment Station, Experiment, Georgia died January 20, 1969, following a brief illness. He was 71 years old.

He was associated with the Experiment Station for 38 years prior to retiring in 1965, and was for many years Head of the Chemistry Department. His research in peanut curing and utilization resulted in an impressive total of 47 publications in this field.

In addition to his membership in the AOCS, he was a member of the American Chemical Society (Chairman of the Georgia Section), New York Academy of Science, American Institute of Chemists, and a Fellow of the American Association for the Advancement of Science.