0.05 0.10 MOLE FRACTION CH<sub>3</sub>-R Figure 1. Yields of CH<sub>3</sub><sup>18</sup>F vs. mole fraction of substrate in SF<sub>6</sub>: □, (CH<sub>3</sub>)<sub>4</sub>Sn; ○, (CH<sub>3</sub>)<sub>5</sub>SnH; ●, (CH<sub>3</sub>)<sub>4</sub>C. CH<sub>3</sub><sup>18</sup>F yield actually increases with decreasing substrate concentration, as shown in Figure 1. The

 $CH_{3}$ <sup>18</sup>F yield from <sup>18</sup>F reaction with neopentane, on the other hand, displays the typical behavior of a "hot" product extrapolating to zero yield at high dilution in SF<sub>8</sub>. The failure of the  $CH_{3}$ <sup>18</sup>F yield to diminish with decreasing alkyl tin concentration indicates that an overwhelmingly large fraction of the substitutions in (1) is initiated by *essentially thermal* <sup>18</sup>F atoms.<sup>8</sup> Since abstraction of H by a fluorine atom occurs on nearly every collision with alkyl groups,<sup>3,4,9</sup> the efficiency of displacement of SnH(CH<sub>3</sub>)<sub>2</sub> or Sn(CH<sub>3</sub>)<sub>3</sub> on carbon must be quite high and roughly proportional to the

(8) The term "thermal" implies a Maxwell-Boltzmann distribution of fluorine atoms at the 10° temperature of the system. For species such as atomic fluorine which react on nearly every collision with some substrates, the maintenance of a true *thermal* distribution is often quite difficult. For us "essentially thermal" means roughly that >95% of the <sup>18</sup>F atoms have <1 kcal/mol of kinetic energy at reaction.

(9) K. H. Homann, W. C. Solomon, J. Warnatz, H. G. Wagner, and C. Zetzch, Ber. Bunsenges. Phys. Chem., 74, 585 (1970).

number of Sn–C bonds. The activation energy for this substitution process must, therefore, be  $\leq 1 \text{ kcal/}$  mol. Indeed, the noticeable upward trend in CH<sub>3</sub><sup>18</sup>F yield with diminishing substrate concentration suggests that the activation energy for this substitution is slightly less than that for H abstraction from the molecules (but for both reactions  $\leq 1 \text{ kcal/mol}$ ).

The cleavage of Sn–Sn bonds by F atoms has been suggested previously in explanation of the formation of  $(CH_3)_3SnF$  in uv-irradiated  $(CH_3)_3Sn-Sn(CH_3)_3$ mixtures with  $C_2F_4$ .<sup>10–12</sup> Such a mechanism is qualitatively consistent with our present results but does not seem quantitatively capable of explaining the high yields of  $(CH_3)_3SnF$  actually found, for the great majority of F atoms formed in such a mixture would be expected to react by other pathways: abstraction of H atoms with the formation of HF,<sup>3,4</sup> or addition to  $C_2F_4$ . No comparable experiments involving cleavage of Sn–C bonds by F appear to have been performed.<sup>12</sup>

The free-radical chain attack of bromine atoms on  $R_4Sn$  has been presumed to go first with the displacement of R to form  $R_3SnBr$ , followed by the attack of the displaced R on  $Br_2$  to form  $RBr.^{13}$  However, the identifiable products would be the same if the first step were displacement of Sn on C with the formation of RBr, followed by the attack of  $R_3Sn$  on  $Br_2$  to form  $R_3SnBr$ . The two sequences can only be distinguished by experiments in which the initial radical source and the radical terminator (both  $Br_2$ ) are not identical. The generality of these displacement reactions at Sn-C bonds is now being tested with other substrates.

(10) M. A. A. Beg and H. C. Clark, *Chem. Ind. (London)*, 76 (1960).
(11) H. C. Clark, J. D. Cotton, and J. H. Tsai, *Can. J. Chem.*, 44, 903 (1966).

(12) K. U. Ingold and B. P. Roberts, "Free-Radical Substitution Reactions," Wiley-Interscience, New York, N. Y., 1971, pp 96-107.

(13) S. Boué, M. Gielen, and J. Nasielski, J. Organometal. Chem., 9, 443, 481 (1967).

(14) This research was supported by AEC Contract No. AT(04-3)-34, Agreement No. 126.

John A. Cramer, R. Subramonia Iyer, F. S. Rowland\*

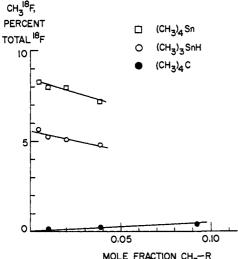
Department of Chemistry,<sup>14</sup> University of California Irvine, California 92664 Received October 27, 1972

## Book Reviews\*

**Chemical Substructure Index (CSI) 1970** (2 volumes). Institute for Scientific Information, Philadelphia, Pa. 1971. xix + 2722 pp. \$1000.00 (includes 11 monthly indexes as well).

This brave venture represents a major commitment to provide a literature-searching tool for chemists that is properly described as unique. It is an index to new compounds reported in *Current Abstracts of Chemistry* and *Index Chemicus* (CAC and IC) during the year. The special feature that justifies the existence of such a work is that it is not an index of names, but of line-notation structures, a characteristic that greatly increases the power of the permuting method for bringing common structural features together.

Line notations can be quite easy to read, and no one should allow himself to be put off by an imagined great barrier. The Wiswesser notation (WLN) used in this index can be more quickly learned than can systematic nomenclature, and, indeed, the simple elements needed to make use of the CSI can be picked up in less than an hour (a table of the WLN code symbols for the principal functional groups is included). Thereafter, one can confidently locate all new compounds having a given functional group, regardless of what else may be present, by looking under only a single heading. Under "KO," for example, all compounds containing the amine oxide function can be found, even though the KO portion of the line notation may ordinarily be buried in the middle. If one further restricts his interest to amine oxides containing a carbonyl group in addition, it is simple to use the "Quikscan" column, in which, for each compound, the other functional groups are listed (in WLN) separate from the detail of the code for the carbon skeleton. Having located these by checking off each entry in which the Quikscan includes a V (carbonyl), one can also restrict the search even further, such as, for example, to carbocyclic compounds. If one has become "fluent" in WLN, it may be worth-



YIELD

<sup>\*</sup>Unsigned book reviews are by the Book Review Editor.

while checking each citation for the full structure at this point, but that is not really necessary. The index entries give the abstract number and the compound number for the corresponding CAC and IC abstract, in which the structure will be displayed and the literature reference given.

It should be evident that the CSI is well suited for efficient "manual" (i.e., visual) use, even though the system is also well adapted to computer handling. The publishers claim that theirs is the only means presently available to do substructure searching without computer access, and they appear to be right. The importance of substructure searching can be appreciated if one considers the task of locating all new chloronitriles with the aid of a conventional index. Each parent nitrile (of which there might be nearly a thousand) would have to be looked up separately, and then each major heading would have to be searched laboriously, looking for chloro substituents perhaps buried in other parts of the name. With the permuted WLN index, only one major heading need be consulted, and the search for a second structural feature (e.g., chloro) is greatly facilitated by the "Quikscan" column. The value to a research laboratory, both in time saved and capital investment avoided, could be substantial.

It is natural to ask how this new index relates to Chemical Abstracts Annual Index. They complement each other; each does much that the other cannot. The CSI covers only *new* compounds and has entries only for initial reports, not of new information on previously reported compounds. It does not separately refer to types of reaction, to uses, to sources, to broad classes (*e.g.*, "detergents," "vinyl polymers"), to methods, etc., all of which topics can be found in Chemical Abstracts Indexes. The CSI is thus a new tool, with a new function, and broadens the capability of the research chemist. It is too early to tell if this service will be found worth the substantial cost, but the publishers are evidently staking a great deal on their conviction that it will. It deserves a serious, sympathetic, yet critical trial.

Organometallic Compounds. Volume III. Compounds of Arsenic, Antimony and Bismuth. Second Edition, First Supplement. Edited by M. DUB (Monsanto Co.). Springer Verlag, New York, Heidelberg, Berlin. 1972. xxi + 613 pp. \$24.80.

The editor has attempted "to achieve a complete coverage of the scientific and patent literature" for the period 1965–1968. This material is presented in highly abbreviated form, ordered according to structural type, analogous in principle to the arrangement of Beilstein although different in execution. The entries give methods of synthesis, physical constants, and reactions; the literature references, which number 1661, are collected at the back of the volume. There is no index, but a detailed table of contents makes it not difficult to locate what one is after. A thoughtful feature is the inclusion of a separate bibliography of Review Publications and Monographs (there are 27). The amount of activity in this somewhat esoteric field should be surprising to the uninitiated.

Proceedings of the Second Lunar Science Conference. Volume 1: Mineralogy and Petrology. Volume 2: Chemical and Isotope Analyses. Volume 3: Physical Properties. Edited by A. A. LEVINSON (University of Calgary). The MIT Press, Cambridge, Mass. 1971. Vol. 1, xiii + 986 pp. Vol. 2, xi + 966 pp. Vol. 3, x + 866 pp. \$25.00 per volume (\$70.00 per set).

These volumes contain the papers presented and are rich in photographic illustrations, both in color and black and white. The large number of papers contain a mass of detailed information of potential interest to inorganic, physical, and analytical chemists. Each volume has an author index, but the lack of a subject index makes it laborious to retrieve specific information, for which one would have to scan the tables of contents.

**PVC Technology.** Third Edition. By W. S. PENN. Revised and edited by W. V. TITOW (Yardley Laboratories) and B. J. LANHAM (James Ferguson and Sons, Ltd.). Wiley-Interscience, New York, N. Y. 1972. xii + 545 pp. \$39.95.

In this edition, eight of the 29 chapters have been rewritten, and other material has been brought up to date. The book is meant to be both a general guide for the nonspecialist and a reference book for "the skilled technologist" and seems to fulfill the intention. Each chapter is accompanied by a short list of references to books, patents, symposia, and journals (but none could be found to this journal).

Fundamentals of Organic Chemistry. Theory and Application. By GEORGE B. BUTLER (University of Florida) and K. DARRELL BERLIN

(Oklahoma State University). The Ronald Press Co., New York, N. Y. 1972. ix + 1113 pp. \$16.50.

This textbook is primarily designed for a one-year undergraduate organic chemistry course. The first 14 chapters are intended for the first semester. Chapters 1 to 3 constitute an introduction to organic chemistry: structure, bonding, and electronic effects in organic compounds. Chapters 4 to 13 cover what the authors call "The Vocabulary of Organic Chemistry," functional groups. These ten chapters are basically broken down into five topics: structure, nomenclature, methods of preparation, chemical reactions, and uses. The second semester covers some of the more theoretical aspects of organic chemistry: energy relationships, stereochemistry, reactions and reaction mechanisms, cations, anions, free radicals, and electron-deficient neutral intermediates such as singlet and triplet carbenes, nitrenes, and arynes.

The last four chapters deal with complex structures such as nonbenzenoid aromatics, polycyclics, carbohydrates, and macromolecules. After each chapter, a list of references for suggested reading is given, and a problem set is given which includes a few challenging problems.

A few subjects presented in the text are sometimes omitted from a one-year undergraduate organic chemistry course: for example, singlet and triplet carbenes and nitrenes.

In general, the book is readable, and the terms and concepts which appear in the text are well defined and illustrated. This book could be used in a beginning organic chemistry course by students regardless of their major.

## Clayton B. Quinn, University of Michigan

Electron Spin Resonance. By J. E. WERTZ (University of Minnesota) and J. R. BOLTON (University of Western Ontario). Mc-Graw-Hill, New York, N. Y. 1972. xiv + 497 pp. \$22.50.

The authors have written an excellent introductory text on electron spin resonance with 14 chapters and 4 appendices. It begins with an introductory chapter which presents several quantum mechanical concepts, and follows this with a short discussion of instrumentation. Most of the remaining chapters deal with static problems such as calculation of energy levels and transition probabilities. In addition there are two chapters devoted to dynamic phenomena, such as relaxation, line widths, and double resonance.

The longest discussion, one quarter of the book, is devoted to transition metal ions in solids. The major emphasis here is on first row series ions, and each orbitally degenerate and orbitally nondegenerate ground state case is treated explicitly. The final section (12.7) on the practical interpretation of spectra is particularly helpful.

The next longest topic, 20% of the text, treats free radicals in solids. The emphasis is on the anisotropies in organic free radicals formed by irradiation. Inorganic radicals are also discussed. In addition there is a lengthy discussion of free radicals in solution and of triplet states. The section on gaseous free radicals seems misplaced in the transition metal chapter.

A final short chapter on biological applications gives a good summary of the main problems of interest to research workers. This is particularly timely because so many magnetic resonators are currently becoming interested in biological problems.

The text ends with appendices on (A) mathematical operations, (B) angular momentum, (C) hyperfine calculations, and (D) spectrometer performance. Useful tables of physical constants, conversion factors, and nuclear moments are printed on the inside covers.

This volume should be extensively used as a text in introductory electron spin resonance courses in both chemistry and physics departments, and perhaps in some biology departments. It starts at the beginning and develops the theory without presupposing specialized background knowledge. The level is sufficiently high to prepare the student for reading standard publications in the current literature and advanced treatises such as Abragam and Bleaney's "Electron Paramagnetic Resonance of Transition Ions."

Charles P. Poole, Jr., University of South Carolina

Systematic Analysis of Surface-Active Agents. 2nd Edition. By MILTON J. ROSEN (Brooklyn College of the City University of New York) and HENRY A. GOLDSMITH (Turco Products Division, Purex Corporation). Wiley-Interscience. New York, N. Y. 1972. xxvi + 591 pp. \$27.50.

This revised edition (First Edition, 1960) is a greatly expanded, up-to-date laboratory manual and reference volume on the analysis of surface-active agents. The five chapters (Classification, Detection and Isolation, Separation of Mixtures, Structural Analysis and Identification, and Quantitative Analysis) describe a systematic approach to the analysis of unknown surfactants, as well as the more usual testing of known materials. A section on the separation and identification of surfactant raw materials is also included. Most of the new material in this edition is on instrumental methodology, notably infrared and nuclear magnetic spectrometry for determining molecular structure, and chromatographic methods for separations and quantitative determinations. New tables in the Appendix include a compilation of ir spectra of representative surfactants, and a table of recommended packings for gc columns. The volume is of value to everyone engaged in surfactant chemistry.

Irving I. Domsky, Armour-Dial, Inc.

4. Internationales Symposium. Biochemie und Physiologie der Alkaloide. Halle (Saale), 1969. Edited by H. R. SCHÜTTE, D. GROSS, H.-W. LIEBISCH, and U. STEPHAN. Akademie Verlag, Berlin (DDR). 1972. 550 pp. 110 Marks.

This book records lectures, papers, and discussions at the 4th International Symposium on Biochemistry and Physiology of Alkaloids, held in the DDR in mid-1969. The scope of the meeting was interestingly broad, ranging from purely chemical studies to strongly biologically oriented work in many fields of alkaloid chemistry. Structure determination, organic synthesis, biosynthesis, enzyme studies, biochemical systematics, plant physiology, and other specializations are represented. What a pity it is, then, that this book has by now lost much immediate interest, owing to three years' delay in its publication. Such a delay is disastrous for a book like this, but it still is interesting to read and has some useful reference material. Inclusion of verbal discussions which took place at the meeting seems to me to be generally unnecessary.

P. W. Le Quesne, University of Michigan

Modern Food Analysis. By F. L. HART and H. J. FISHER. Springer-Verlag, New York, N. Y. 1971. 519 pp. \$32.00. "Modern Food Analysis" by F. L. Hart and H. J. Fisher is an

"Modern Food Analysis" by F. L. Hart and H. J. Fisher is an ambitious attempt to combine an up-to-date compendium of methods of analysis with discussions of the history and methodology of processing foods and beverages; extensive data of their composition; and a complete survey of standards and specifications including legal standards for foods in the United States and Canada, government marketing specifications, and voluntary standards adopted by trade associations.

This is a big book, well over 500 pages, and an expensive one. To justify such an expenditure, the book must satisfy the needs of those for whom it is expressly intended; namely, according to the publishers, food chemists, quality control personnel, and regulatory officials as well as postgraduates in chemistry and food technology. And the common focus of interest shared by the potential users is assumed to be the methods of analysis.

It is difficult to assess the usefulness of any methods book without in fact first putting it to test in the laboratory. This one, however, seems unduly inconvenient. The format is such that it would be extremely difficult to follow a procedure directly from the text. As it is obviously not designed to be used as a laboratory manual, anyone wishing to exploit the "cookbook" aspects would have to first transcribe the method of interest to a more convenient form.

A more serious criticism is that the book suffers from redundancy as many of the methods are taken directly from standard sources, in particular the "Official Methods of Analysis of the AOAC," presumably already in the possession of food analysts. One finds, for example, that the analytical procedures for milk include twenty AOAC methods, and only seven from other sources.

The title, "Modern Food Analysis," and date of publication, 1971, lead one to expect extensive coverage of recent developments. In fact, literature citations more recent than 1968 are virtually impossible to find, and many are ten to twenty or more years old. Where the authors could have contributed significantly by providing detailed consideration of the exciting new analytical tools and techniques, they resorted to rather cursory mention of them, leaving the reader with the task of finding detailed explanations elsewhere, and possibly at great inconvenience.

The descriptive material is for the most part superficial and inadequate, hardly at a level sutitable for professional analysts or graduate students. When, in addition, inaccuracies are found, then credibility of the text becomes questionable. One example can be found on page 10 where the statement appears that nearly all foods are essentially nitrate-free. The present concern about spinach and beets as food for infants because of their high nitrate content belies this statement. The discussion of the procedure for roasting and blending coffee on page 93 ignores the prevalent practice of many roasting plants where blending precedes roasting with the composition of the blend predetermined.

Many tables are interspersed throughout the text, some identified by number and title, others not. The rationale for tabulating certain information is sometimes obscure; why, for example, the extensive tabulation of analytical data of citrus fruits from past seasons going as far back as the 1920's (pp 246-249)? Also, it is apparent that the presentation of data has not been carefully checked for consistency, when energy value is expressed as cal/100 g in Tables 10-1, 10-2, 10-5 (pp 180, 181, 186) and as fuel value per pound, cal in Table 10-6 (p 202).

Evidence that the book has not been particularly carefully edited to bring it up-to-date is indicated by the persistence of the use of  $m_{\mu}$  rather than the now generally accepted nm for wavelengths of light, and the failure to correct the statement on p 53 that a mixture of cyclamate and saccharin is preferred over either sweetener alone in artificially sweetened beverages, although the authors have indicated elsewhere their awareness of the regulation banning such action (p 324).

Finally, for a book intended for chemists, but singularly devoid of chemical formulas, it seems a particular shame that the two structural formulas that are given ( $\beta$ -carotene and vitamin A, pp 457 and 458) should be mislabeled.

Undeniably, a comprehensive modern text on food analysis is needed. This reviewer is not convinced that the present volume fills that need.

Angela C. Little, University of California-Berkeley

Poly(Vinyl Chloride): Formation and Properties. Edited by B. SEDLACEK (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences). Wiley-Interscience, New York, N. Y. 1971. vii + 369 pp. \$14.50.

This book is a compilation of 33 of 53 papers presented at the Seventh Microsymposium on Macromolecules held under the auspices of the International Union of Pure and Applied Chemistry at Prague, Sept 7–10, 1970. The papers relate to seven thematic groups: (1) radical polymerization, (2) nonradical polymerization, (3) morphology and mechanical properties, (4) rheology and plasticization, (5) solution properties, (6) molecular structure, and (7) destruction.

Rather than being a reference text on PVC, the book represents a scan of the thinking and research work of many well-known and capable experts in the field. The major fields of interest discussed are (1) the physical and mechanical properties of PVC and (2) degradation studies of PVC. The subject matter is considered to be a worthwhile addition to the library of anyone having an interest in these fields.

E. S. Smith, The Goodyear Tire & Rubber Company

Analytical Profiles of Drug Substances. Volume I. Edited by KLAUS FLOREY. Academic Press, New York, N. Y. 1972. xi + 480 pp. \$14.00.

As implied by the title, this book is the first volume of a series designed to supply relevant background information for analysis of official drugs. The format used treats each drug as a separate chapter and supplies information concerning physical properties including nmr, ir, uv, mass, and ORD spectra; chemistry (synthetic and behavioral); and analytical methods and biochemistry of each drug in outline form. Twenty-one drugs are covered in this volume.

Data and information are consolidated from diverse formal publications as well as from authoritative unpublished sources so as to provide a fairly complete "profile" on each drug.

Despite certain deficiencies which include loose terminology, *i.e.*, "DSC Spectrum" and in some cases documentation of data without apparent reason, the authors have significantly benefited the area of drug analysis.

This volume, as well as the series, will provide primary reference material and help to fill an existing void.

Dale H. Szulczewski, Parke, Davis & Company