Computer Software Reviews

PAPYRUS. Version 7.0. Research Software Design: 2718 SW Kelly St., Suite 181, Portland, OR 97201. Voice: (503) 796-1368. FAX: (503) 241-4260. E-mail: RSD@applelink.apple.com. List Price $99.00; Demo system $25.00.

Papyrus Version 7.0 remains the versatile bibliography database and formatter it was when we reviewed Version 6.0 about 4 years ago. Its main feature is the ability to input a list of references from database searches and reformat selected ones to meet the requirements of the particular publication for which you are writing. References may be typed in, imported from various on-line databases, or copied from word processor files. While importing, the program distinguishes among journal articles, books, reports, patents, and other types of references, as long as you have accurately described the formats for each of these and the formats are scrupulously followed in the list being imported. Papyrus comes with an extensive group of import formats already prepared for this purpose, as well as formats for exporting references in the preferred style of many journals. A new feature of the program is the ability it gives of adding one or more "index cards" to any reference, so that extensive quotes and comments can be stored with it. Several additional data fields describing a reference, including three user definable fields, are included in Version 7.0. The program can also "winnow" the database, that is, search it to clear out duplicates.

This version works with Windows, although it runs under DOS. As you work on a document in your word processor, you can pop into Papyrus and select a reference, and it will then place a code into the document. Lists of keywords and abstracts help in the selection of the correct reference. When the document is finished, Papyrus will process it into a new document with the codes converted into reference numbers, in your specified format, placed at the appropriate places in the document. Then it will produce a file listing the references, to be appended to the document as the bibliography. With Windows based word processors (Word, WordPerfect, and WordStar), the code for each reference is put into the clipboard for pasting into the document.

Unfortunately, the new version still has the look and feel of five-year-old software. If you routinely use Windows software, you may feel that there are just too many times when you have to refer to the manuals and type cryptic codes. On the other hand, the manuals are literate and helpful. If you have already developed an extensive Papyrus database, the additional information which you can store with each reference in this version may make the upgrade useful. However, a database or even a word processor program may suffice to keep your lists of references, although transferring large numbers of references into a database program may require a lot more hand labor than Papyrus would.

The licensing terms are very reasonable. You may copy and give away the Demo program, included in the package, but not the full program. As a registered user, you are entitled to develop and use up to four separate databases for each registered copy and, sensibly enough, may copy the program to another computer for your own use. There is a student version available free to registered users, which will work for 120 days and handle up to 200 references. This can be distributed to students in classes such as technical writing. In addition, a "Retriever" version may be freely copied and given away or even sold with your own database. This allows users to search for and print references, although they can make no changes or additions.

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Book Reviews

Flame Chemiluminescence Analysis by Molecular Emission Cavity Detection. Edited by David Stiles (Acadia University), A. C. Calokerinos (University of Athens), and Alan Towshend (The University, Hull). John Wiley and Sons: New York. 1994. xiv + 206 pp. $90.00. ISBN 0-471-94340-1.

Perhaps all of us have been introduced to the qualitative abilities of the "flame test" and possibly have wondered of its quantitative abilities. This volume describes those abilities in earnest. The editors have compiled a comprehensive and current review of the molecular emission cavity analysis (MECA) method concisely in book form. The first two chapters give a brief history of the MECA approach from the early astute observations of Mulder and Salet to the final realization of its quantitative potential in the 1970s. The basic principles, including discussion on the hydrogen/air flame, function of the cavity, and flame spectroscopy, are concisely addressed in Chapter 2. The charming simplicity of the method is evidenced by the use of a steel, socket-head cap machine screw as one variety of sample cavity. But the power and utility of the method is also well demonstrated by this volume. The reader can obtain a basic insight into the approach in a short sitting with this book.

Chapter 3 describes the instrumentation and automation. Cavity design and commercial instruments are well described. A discussion of the application of MECA as a detector for GC, LC, and HPLC is included. Automation is discussed with regard to sample introduction but not multielement analysis.

Chapters 4–7 give a résumé of the application of MECA to the analysis of elemental groups: Chapter 4, the calcogens; Chapter 5, arsenic, antimony, boron, silicon, germanium, and tin; Chapter 6, nitrogen, phosphorus, and carbon compounds; Chapter 7, halogens and metals. The use of indium doping and indium-lined cavities is discussed with regard to the determination of halogens. Interferences by foreign ions are tabulated for many analyses. Indirect methods are also addressed. The reader will welcome the inclusion of the emission spectra for most of the elemental analytes.

The editors are quite pragmatic in their presentation of the method; the volume has many attributes of a handbook for the technique. With this approach, a few academic issues are not covered well. The book lacks discussion of the decision philosophy involved in the choice of detectors and wavelengths of observation. Given the inherently broad molecular emission features, some consideration of overlap and wavelength selection would be useful; indeed, diode array spectrometers are not mentioned at all. Several pages of discourse on the eternal trade off between sensitivity and selectivity would be useful for a emission photometry method such as this.

In spite of these quibbles, I can recommend the monograph to all practically inclined workers in emission spectrometry. The book is Volume 129 in the publisher's series of monographs in Chemical Analysis.

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JA945030E

The Chemistry of Alkanes and Cycloalkanes. By Saul Patai and Zvi Rappoport (Hebrew University of Jerusalem) J. Wiley Interscience: New York. 1992. xiv + 1078 pp. $610.00. ISBN 0-471-92498-9.

The Chemistry of Alkanes and Cycloalkanes sets forth the tradition established in Prof. Patai's series *The Chemistry of Functional Groups*. It is, however, a little unusual for this series in that the alkanes and cycloalkanes cannot be treated as a typical functional group, so that the contents of individual chapters are sometimes not as focused as in earlier volumes.

Richard Bader's opening chapter, for instance, deals with his atoms-in-molecules approach to the analysis of molecular wave functions. It is an excellent introduction to his technique and uses alkanes as examples. It is, however, perhaps a little out of place in this volume. Eiji Osawa's Structural Chemistry of Alkanes is a very personal view (as the author himself points out), where I would have preferred a comprehensive literature survey.

Edgar Anderson's chapter on conformational analysis in saturated hydrocarbons is, in contrast, extremely comprehensive and presents a mine of information on both experimental and molecular mechanics studies in this area. Similarly, Brewster's chapter on chiroptical properties and Cohen and Benson's contribution on the thermochemistry

on alkanes are destined to become standard citations. The following four chapters deal with spectroscopy and analysis of alkanes and are all valuable contributions for active researchers. Aizenshtat deals with the analysis of alkanes, whereas Berger, Gäumann, and Heilbronner deal with NMR, mass, and photoelectron spectra, respectively.

Hopkinson's chapter on the acidity and basicity of alkanes provides an ideal introduction to Olah and Prakash's Electrophilic Reactions on Alkanes. These chapters would have benefited from being published back-to-back, but they are instead separated by Mehta and Prakash Rao's review of modern synthetic methods. This chapter provides a welcome update of the now dated Comprehensive Organic Chemistry articles.

Robert Crabtree's chapter on the organometallic chemistry of alkane activation is very timely but a little too short (24 pages) to do such an important subject justice. Oppenländer, Wang, and Adam, on the other hand, treat alkane rearrangements and photochemistry very comprehensively and also provide an excellent historical overview of such classics as the adamantane rearrangement and the norbornadiene/quadricyclane system.

Chapter 16, on the radiation chemistry of alkanes and cycloalkanes (by Hummel) is a far more specialized contribution that will have less general appeal than many of the other chapters. The same is true of Zieliński and Kańska's contribution on the synthesis and use of isotopically labeled alkanes. These chapters are valuable references for specialists but fail to touch on matters of general interest.

Shäfer's Electrochemical Conversion of Alkanes and Banthorpe's Natural Occurrence, Biochemistry and Toxicology, on the other hand, are readable and full of information of remarkably general interest. They are the sort of review that can be read simply out of interest. This also applies to Agosta's chapter on inverted and planar carbon—a subject that has aroused continued interest over the years. This chapter is likely to become a beloved source of examples for graduate courses in structural organic chemistry. Finally, Glen Russell's review provides an excellent overview of the radial reactions of alkanes, although I would like to have seen this section extended to include the synthesis of alkane skeletons by radical methods.

This volume is, as expected, a valuable reference work. It has perhaps a wider appeal than many others in the series because of the generality of many of the principles that are described here for alkanes and cycloalkanes. The aims, comprehensiveness, and general interest of the individual chapters do vary considerably, but this does not detract from the fact that researchers in the alkane area and many others will find much of value.

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JA9247272

A New Dimension to Quantum Chemistry. Analytic Derivative Methods in *ab initio* Molecular Electronic Structure Theory. By Y. Yamaguchi, Y. Osamura, J. D. Goddard, and H. F. Schaefer III. Oxford: New York. 1994. xxii + 472 pp. $75.00. ISBN 0-19-507028-3.

In their introduction the authors observe that in 1969 Pulay (*Mol. Phys.* **1969**, *17*, 197) proposed the analytic evaluation of the first derivative of the electronic energy with respect to nuclear coordinates, a proposal that has revolutionized *ab initio* quantum chemistry. Their book represents a formal exposition, from a unified perspective, of the advances in analytical derivative theory that have been achieved over the past 25 years. It is oriented toward entry level graduate students or researchers concerned with the details of the theoretical treatment of this problem.

The book develops analytic derivatives of the electronic energy within the nonrelativistic Born Oppenheimer approximation from a consistent formal perspective, with the goal of providing "a systematic presentation of the necessary algebraic formula", a goal that is certainly achieved. The authors consider derivatives of the electronic energy determined from the variational principle. An extensive bibliography and end of chapter citations provide the reader with access to the technical literature.

Chapters are devoted to closed shell, open shell, two configuration, and pair excited self-consistent field wave functions; general multiconfigurational self-consistent field wave functions; and general configuration interaction wave functions. Derivatives through fourth order are considered explicitly. The treatment is exhaustive in its detail; however, the book benefits from an organizational style that focuses on the commonality among the various classes of derivatives so that the pace of the book is paradoxically fast in spite of its detail. The discussions of the key issue of the determination of molecular orbital derivatives—the variety of forms of coupled perturbed Hartree—Fock equations—are exemplary in this regard. The authors are careful to describe the computational implications of the energy derivative equations and provide a cogent discussion of the use of the Z-matrix method (Handy, N. C.; Schaefer, H. F. *J. Chem. Phys.* **1984**, *81*, 5031) to reduce the computational effort required for their evaluation. Chapter 17 considers derivative of the electronic energy with respect to electric field perturbations. The use of this theory as a computational tool to determine electric polarizabilities and dipole moment derivatives is discussed. Consistent with the pedagogical orientation of this book, the use of analytic derivative theory to consider the validity of the Hellmann—Feynman theorem (Hellman, J. *Einfuhrung in die Quantenchemie*; Deuticke: Leipzig, 1937. Feynman, R. P. *Phys. Rev.* **1939**, *56*, 340) is also discussed.

Omitted from the discussion are (i) derivatives of energies based on perturbation theory (such as Møller—Plesset theory) and coupled cluster theory, (ii) the use of energy derivatives in characterizing nonadiabatic processes, (iii) the determination of the basic (atomic) derivative integrals required to implement the formalisms discussed in this work, and (iv) the computational aspects of the implementation of these techniques on modern computer architectures.

As the authors observe, the formalisms described in this volume have enabled the treatment of problems in molecular structure hardly imaginable 25 years ago. Significantly, then, the penultimate chapter in this volume addresses the contributions of analytic derivative theory to quantum chemistry with illustrative examples. The final chapter looks at future directions for research in this vital area of computational chemistry.

In summary, the authors have provided what this reviewer believes to be the reference of choice for introducing a neophyte to the details of analytic derivative methods in electronic structure theory.

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Chemical Analysis by Nuclear Methods. Edited by Z. B. Alfassi (Ben-Gurion University of the Negev). John Wiley & Sons: New York. 1994. xx + 556 pp. $150.00. ISBN 0-471-93834-3.

Nuclear analytical methods are important tools for the modern analytical chemist. They are very sensitive, allowing, in the best cases, detection of single atoms. Many of these techniques, such as neutron activation analysis, radioimmunoassay, and PIXE, are widely used. Because of these factors, the appearance of this new collection of essays about these techniques is welcome.

To place this book in perspective, one needs to note that there are a number of introductory treatments of the basic ideas of nuclear chemistry that are suitable for nonspecialists. (The recent volume by Ehmann and Vance is especially recommended for analytical chemists.) This book is not a substitute for those introductory treatments. To read it and use the information effectively, one must have some prior training and/or experience with nuclear and radiochemistry. Instead, this book is a collection of 20 self-contained articles by experts (mostly from Israel and Europe) about various nuclear analytical techniques. The overall collection is unique, bringing together in a single volume information about a wide variety of methods.

The first five articles review some basic concepts in nuclear and radiochemistry (interaction of radiation with matter, detectors, accelerators, sources, nuclear reactions, and health physics) but are not adequate for the nonspecialist. Five articles deal with various aspects of activation analysis, with essays by Landsberger and Sellschop being particularly good. Three articles treat X-ray based methods; the article on PIXE (particle-induced X-ray emission) is quite informative. The two chapters on the use of radiotracers (isotope dilution analysis and radioimmunoassay) are, in my opinion, the best articles in this collection. Miscellaneous chapters on positron annihilation, Mössbauer spectroscopy, Rutherford backscattering, and other topics round out the discussion.

This book will be a valued addition to any library of up-to-date information on nuclear analytical techniques. Hopefully most libraries will purchase it, although its high cost will be a barrier to many scientists to adding it to their personal libraries.

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