nothing on how to input or define one, unnecessarily adding to the manual-searching/experimentation aspects of programming in a new language. Installation did not exactly follow the written procedure, apparently confusing module additions with the basic language installation, but nothing anyone with a knowledge of DOS will have much trouble with. Included in the manual are five tutorial lessons that do a good job in introducing beginners to GAUSS' divers capabilities. There are some errors in the text, not only here but in the modules as well, mostly of a typographical nature such as neglecting to define one of the variables in a 3D plot. Worse is that it is not always clear when certain procedures or default parameters must be loaded prior to attempting to follow the examples. Most of these problems are cosmetic, especially in comparison to the normal difficulties encountered when using a new programming language and in attempting to perform tasks formerly unattainable on a PC.

GAUSS lets you have full access to DOS and any other programs on disk without leaving the environment, so you can change directories, copy files, even use it to build up batch programs. It is also possible to interface with routines written in Assembler, or C and FORTRAN providing one has a compatible compiler. It even comes with a de-installation program for removing all associated sub-directories from a hard disk and the escape key works.

GAUSS is not copy protected and can be run on a system with two DS/DD drives but is best installed on a hard disk. It requires DOS 2.1 or higher, a math coprocessor, and at least 320K RAM. A CGA graphics card is needed for use of module 1, 512K and any of the standard graphics cards for module 12. Aptech is constantly revising the program(s) and entitles owners to their updates. There is also a GAUSS newsletter, subscriptions are $12.00 per year. It might be difficult to run this program with less than 640K since the program inherently challenges its users to push around large amounts of data, though there are commands in the language for dealing with freeing up previously used memory. Unfortunately, 640K is also the maximum memory utilized regardless of how much is on the system.

The closest competitor of GAUSS is probably PC-Matlab by Math Works, and both have very similar capabilities. Matlab is more expensive, is copy-protected, and does not currently have the graphics output capabilities of Module 12, but it does have a better user interface with good on-line help and parallel versions that run on mainframes as well as the Macintosh. Asyst by MacMillan Software (see *J. Am. Chem. Soc.* **1987**, *109*, 3178) is also more expensive and copy protected, but it more powerful. It has interfacing capabilities for data acquisition and can handle 65 000 elements with up to 16 dimensions per array as compared to GAUSS's limit of 8190 elements and 2 dimensions. The GAUSS language is somewhat easier to learn, but this is subject to the individiual programmer's preference.

In summary, GAUSS is a good programming package of interest to anyone desiring to do serious computation on a personal computer. It is versatile, powerful, fast, accurate, and relatively affordable. These features far outweigh the inconvenience of a scant user interface. If your calculations can stay within GAUSS' array size and memory limitations, it will allow you to push your PC to the best of it's number crunching abilities.

Scott A. Smith, *University of California*

Book Reviews *

Handbook of Polycyclic Aromatic Hydrocarbons. Volume 2: Emission Sources and Recent Progress in Analytical Chemistry. Edited by Alf Bjørseth and Thomas Ramdahl. Marcel Dekker, Inc.: New York. 1985. 416 pp. $95.00 (U.S. and Canada); $114.00 (all other countries). ISBN 0-8247-7442-6

This book updates and expands upon the very useful first volume. It consists of eleven chapters, by widely recognized experts, covering most of the current areas of activity in this field. The extensive chapter by S. A. Wise on HPLC updates his chapter in Volume 1. It provides extensive data sets, comparisons of HPLC and GC/MS data on U.S. National Bureau of Standards Standard Reference Materials, and Figure 7, which reproduces the HPLC chromatogram of eleven pentacyclic $C_{22}H_{14}$, is a delight to those of us who have hitched our fortunes to this technique. The Chapter by K. D. Bartle updates the GC chapter in Volume 1. It emphasizes advances in open tubular column GC and expands upon higher molecular weight polycyclic aromatic hydrocarbons (PAH) and derivatives such as nitro-PAH which are commanding increasing attention. The introductory chapter by Bjorseth and Ramdahl on Sources and Emissions of PAH is valuable not only as a literature compendium but also because of the balanced and introspective nature of the review which points up inconsistencies and uncertainties in reporting emissions, for example, in the selection of specific PAH and the definition of total PAH. Bjørseth has also co-authored a later chapter wth G. Becher concerning Determination of Occupational Exposure to PAH by Analysis of Body Fluids. This is an important current area and the authors nicely provide discussion of the pathways PAH follow in living animals and humans. One wishes that there was also discussion of the recoveries of the metabolites in human urine using their technique. Three chapters on PAH emissions from sources [Coal-Fired Plants (K. Warman), Biomass Combustion (T. Ramdahl), and Automobiles (U.R. Stenberg)] follow the first chapter. The eighth chapter on Analysis of 6-Nitrobenzo(*a*)pyrene in Mammalian Cells and Microsomes by HPLC is a departure in style in that it is more specific, using this compound as an archetype for other nitro-PAH. We now know that 1-nitropyrene, 2-nitropyrene, and 2-nitrofluoranthene are considered to be more significant atmospheric mutagens. Chapter 9, by D. W. Later, concerns Nitrogen-Containing Polycyclic Aromatic Compounds in Coal-Derived Materials and concerns azaaromatics as well as amino- and cyano-PAH rather than nitro-PAH. The following chapter by Van Cauwenberghe concerns Atmospheric Reactions of PAH and is well organized and summarized including differences in particulate- and gas-phase reactivities. This Reviewer wishes that a bit more was done to explain the relationship between molecular properties of PAH (besides Free Valence) and reactivity; there is interesting discussion in the 1980/81 literature of the relation of Diels–Alder reactivity of PAH with the gap between the first two ionization potentials of the PAH. The final chapter by Karcher, Reference Materials for the Analysis of Polycyclic Aromatic Compounds, advertises the PAH standards available from the Commission of the European Communities and provides useful discussion on preparation, purification, and purity criteria.

Although this book was published in 1985, it is still very current and will be a useful addition to institutional libraries and the bookshelves of research practitioners. One wishes that there was also coverage of "biologically driven" analysis of pollutants (e.g., by Ames assay) which has indicated the importance of polar derivatives, analysis of indoor PAH, and analysis of PAH metabolite/DNA adducts, but perhaps these will appear in a future volume.

Arthur Greenberg, *Chemistry Division, New Jersey Institute of Technology*

Food Chemistry. By H. D. Belitz and W. Grosch. Translation from the second German edition by D. Hadziyev, University of Alberta, Edmonton, Canada. Springer Verlag: New York. 1987. 774 pp. $79.50.

Few textbooks on Food Chemistry treat the subject as exhaustively as the above-named one. The table of contents is complete enough to give one a thorough idea of what is discussed in the book. Equally detailed is the index. An "Appendix of Selected References to the Literature of Food Chemistry and Related Fields" will be of help to students, especially those entering the field.

Organization of the text follows, more or less, the traditional format. The contents may be divided into sections as follows: Section I, chemical components of foods (water, amino acids, peptides, proteins, enzymes, lipids, carbohydrates, aroma substances—a complete chapter is devoted to each of the above-named topics); in section 2, Chapters 10–18 deal, in consecutive order, with major food products (milk and dairy products, eggs, meat, fish and other aquatic animals used as food, fats and oils, cereals and cereal products, vegetables and their products, fruits and their products); section 3 is composed of four chapters—Chapter 19 discusses sugars, sugar alcohols and honey while alcoholic beverages are treated in Chapter 20, and coffee, tea and cocoa are dealt with in Chapter 21 and spices, salt and vinegar in Chapter 22.

Although Food Science and Food Chemistry are undergoing rapid and dynamic developments, the book is quite up to date, granting time lapses for translation and publication. The very brief preface presents some useful definitions of foods, Food Chemistry, etc., and stresses the im-

*Unsigned book reviews are by the Book Review Editor.

portance and amplitude of the discipline. Chapter 5 could have been more logically placed after Chapter 7, and Chapter 9 seems to be more suited for the closing chapter of the book. As in most of the textbooks on Food Chemistry, the basic biochemistry of food components is covered in great details. This information belongs, logically, to a course in general biochemistry, but since Food Science and Food Chemistry students have such diverse backgrounds, such a treatment can be defended.

This is a well organized text suitable for use by advanced undergraduates and by graduate students in Food Science, Food Technology, nutrition, and related fields. Teachers and researchers will find it to be a useful source of information. It is easy to read and the material is systematically presented. The price is quite reasonable for a rigid, hard-cover book of its size and technical depth.

Horace D. Graham, *University of Puerto Rico*

Stemming the Tide—Arms Control in the Johnson Years. By Glenn T. Seaborg (University of California, Berkeley) with Benjamin S. Loeb. Lexington Books (D. C. Heath and Company): Lexington, MA. 1987. xxi + 495 pp. $24.95. ISBN 0-669-13105-9.

Nobel laureate Seaborg has long combined eminent research in science with distinguished service to his country. From 1961 to 1971 he was chairman of the Atomic Energy Commission, and *Stemming the Tide* deals with events during the Lyndon Johnson presidency, in many of which Seaborg was a participant. The book, rich in detail and including some material not previously made public, is based on Seaborg's daily diary, on official letters and papers during his AEC tenure, on archival materials in the Johnson Library, and on appropriate secondary sources. Benjamin Loeb, his former assistant, again joins him in authorship; earlier the two wrote, on a related topic, *Kennedy, Khruschev and the Test Ban* (University of California Press, 1981). Both volumes give first-hand accounts of important aspects of post WW-II arms developments.

Johnson's presidency began amidst tragedy and, for him, ended in great personal disappointment. Now most readily remembered for his Great Society program, launched while the war in Vietnam escalated, and for continuing that tragic Asian military involvement, he is rarely recalled for his substantial contributions to the advancement of arms control. Yet work toward it continued, albeit at an irregular pace, throughout these years. Building upon the Limited Test Ban Treaty to which Khruschev and Kennedy agreed following the Cuban missile crisis, the President and his staff, with much hard labor, fashioned the Strategic Arms Limitation Treaty—SALT I—just before leaving the White House. At the last moment, agreement on SALT I was frustrated by Russian invasion of Czechoslovakia (August 1968); it remained for the incoming Nixon administration to obtain a final compact.

Johnson set out his arms-control aims early in his presidency in a letter to Chairman Khruschev (January 18, 1964): "to prevent the spread of nuclear weapons: to end the production of fissionable material for weapons; to transfer large amounts of fissionable materials to peaceful purposes; to ban all nuclear weapons tests; to place limitations on nuclear weapons systems; to reduce the risk of war by accident or design; and to move toward general disarmament." As the authors comment, the "continued pursuit of these objectives, with some variations, provides the subject matter of this book."

Russia exploded its first atomic device in 1949. America responded in the 1950s with an unprecedented expansion of fissionable material production and weapon development. By the 1960s this nation was faced with an embarrassment of overproduction and overconsumption of power and resources unless this sorcerer's apprentice could be halted. To stop it, however, meant loss of jobs, political crisis, and an economic nightmare. In an effort to make nuclear energy politically and publicly acceptable, our government sought peaceful uses for it in addition to generation of electric power. One such program was the Plowshare project, discussed at some length. In the end, after the expenditure of much time and money, inescapable nuclear contamination condemned to oblivion this plan for excavating canals and for releasing natural gas trapped in impermeable formations.

As other countries—Great Britain, France, and China—joined the nuclear club and more threatened to do so, nonproliferation became an important political objective. Tentative agreement for a limited test ban treaty finally came about after the idea of test bans and monitoring of tests were argued.

Reading this book in the autumn of 1987 in the aftermath of the Iran/Contra hearings and as we await agreement to moderate the nuclear threat in Europe and look anxiously toward the Middle East, one can only conclude that things in Washington have hardly changed over the years. In the 1960s, as the volume makes manifest, agencies and officials warred among themselves and kept information and secrets from each other. Bureaucracy moved with glacial speed. Foreign governments posed endless problems. Only a continuing willingness to work toward a desirable goal, despite disagreements and disappointments, kept arms control then as now from extinction. Seaborg and Loeb note "...what has been apparent in other presidencies...significant arms control achievements can be brought about only when the president takes a personal and affirmative interest."

Members of the wartime atomic scientific community, having conceived and gestated the atomic bomb, were the first to advance ideas of arms control. Seaborg's books make evident the strong and continuing interest of scientists in peaceable uses of atomic power.

Andrew Patterson, Jr., *Yale University*

NMR Spectroscopy Techniques. Practical Spectroscopy Series. Volume 5. Edited by Cecil Dybowski and Robert L. Lichter. Marcel Dekker: New York. 1987. 384 pp. $89.95 (U.S. and Canada); $107.50 (all other countries). ISBN 0-8247-7441-8

This volume consists of a series of chapters contributed by a number of authors selected for their expertise in the various branches of NMR spectroscopy. The intention is to provide beginning students or practicing researchers with the background requisite for a practical utilization of this valuable tool. The introductory chapter assumes no familiarity with modern pulse-NMR techniques. This is followed by chapters on relaxation processes, 2-D NMR, methods of spectral simplification that do not require 2-D NMR, approaches to structure assignment once the required spectra are obtained, the NMR of solids, and the characterization of polymers. Throughout, the intention is to provide operational (or practical) information without becoming bogged down in mathmatical considerations.

The multiauthor treatment is susceptible to breakdowns in communication and coverage between authors. The editors in this case have done an excellent job of preventing this, and their product achieves the goals they have set for the volume. Which is not to say that all is perfect. Thus, tip angle in Chapter One becomes flip angle in Chapter Three and neither term is very well defined. The relayed coherence-transfer experiment is briefly discussed, but the concept of coherence or coherence transfer is never introduced. These are, however, minor detractions to a useful text.

William B. Smith, *Texas Christian University*

Modern Gas Kinetics. Theory, Experiment and Application. Edited by M. J. Pilling (University of Oxford) and I. W. M. Smith (University of Birmingham). Blackwell Scientific Publications: Oxford. 1987. x + 347 pp. $40.00. ISBN 0-632-01615-9

This book is a polished extension of lecture notes from a course on gas-phase kinetics that was held in the summer of 1985 at Cambridge, and it provides a broad survey of current activities in the field. The book is divided almost equally among sections entitled Theories of Elementary Reactions, Kinetics and Dynamics of Elementary Reactions, and Kinetics of Complex Reactions. Each section consists of several well-written chapters by experts who are active researchers.

After a general introduction to the whole field of gas kinetics by J. P. Simons, theories of chemical kinetics are discussed by M. S. Child, I. W. M. Smith, and G. Hancock. In this section, it is particularly clear that the book presents a broad survey and introduction to the literature, rather than a pedagogical exposition. Topics briefly described in this section include the basic ideas behind potential energy surfaces, classical mechanics, transition-state theory, tunneling, quasiclassical trajectory calculations, state-to-state reaction kinetics, molecular beam dynamics, and unimolecular reactions.

The section on elementary chemical reactions consists of chapters written by G. Hancock, J. P. Simons, and M. J. Pilling. The topics covered include experimental methods for initiating and following chemical reactions in bulk systems, as well as state-selective methods useful in molecular beams. The chapter on the analysis of experimental data is particularly useful, since it fills an important need that is neglected in most kinetics textbooks. Examples are given in each chapter, and the final chapter of this section gives further examples of interesting reaction systems.

The final section is made up of chapters written by R. A. Cox, M. J. Pilling, and J. P. Simons and it describes some of the most important applications of kinetics, including atmospheric chemistry, combustion, lasers, and hydrocarbon cracking. One chapter describes numerical integration of complex kinetics mechanisms and discusses some of the principles of sensitivity analysis.

For those who already have a knowledge of kinetics, this book makes very interesting reading, since it draws together so many diverse strands of current research and helps to place them in perspective. Each subject discussed has its own rich literature; the primary objective of this book is to present only the main ideas, place them in context, and give some important literature references. For those wishing to broaden their kinetics horizons and for those teaching kinetics courses, this book is highly

recommended.

John R. Barker, *The University of Michigan*

Theory of Magnetic Resonance. By Charles P. Pool, Jr., and Horatio A. Farach (University of South Carolina). John Wiley & Sons: New York. 1987. xvi + 359 pp. $59.95. ISBN 0471-81530-6

This book presents an intermediate-level introduction to magnetic resonance theory on the level of spin matrices with a decided slant toward EPR rather than NMR. A strong point of this book is its very clear description of the two-spin system in the general case as well as for NMR and EPR. These three chapters comprise one of the best descriptions of this fundamental case I have ever seen. Similarly, the extensions of the theory to anisotropic Hamiltonians and to systems of more than two spins are very good indeed. The second half of the book is devoted to selected topics in magnetic resonance with an emphasis on EPR techniques and relating magnetic resonance parameters with group theory. There are sections on Mössbauer spectroscopy, spin labels, acoustic, muon, and optical magnetic resonance that could be omitted, and the chapter on Fourier transform NMR is too brief to be worthwhile. NMR relaxation theory is not adequately represented.

This book could be used as a basis for a course in either EPR or NMR with a close following of the text for the basic theory. The book would need to be supplemented from other sources, primarily the literature, for currently popular techniques such as two-dimensional NMR, pulsed EPR, and multiple quantum spectroscopy. The first eight chapters would be a fine beginning for the first half of a course in two-dimensional NMR, for example, with a follow up from the literature. One can only wish that the authors' clear and careful presentations also included product operator formalism, multiple quantum spectroscopy, and modern NMR none of which are currently available in a book suitable for an intermediate level course.

Philip Bolton, *Wesleyan University*

X-ray Methods. By Clive Whiston (Wolverhampton Polytechnic, U.K.). John Wiley Sons: New York. 1987. xxii + 426 pp. $27.95. ISBN 0-471-91387-1

This monograph is part of the British-based *Analytical Chemistry by Open Learning* (ACOL) series edited by F. Elizabeth Prichard. The purpose of the series as stated in the prologue of the text is to provide suitable material in topics in analytical chemistry to what is referred to as "Distance Learners", i.e., the nontraditional audience that is not in attendance at academic institutions, seminars, or forums. The point is quickly and emphatically made that this material is no substitute for supervised lab experience and this point is sufficiently rementioned throughout the text. There are apparently a number of institutions in the U.K. that do offer practical support as a companion to the topics in this series. The material is presented as appropriate to the technician level.

The author has chosen to discuss the two X-ray techniques most prevalent in commerical use: powder diffraction and fluorescence. The instruments discussed and contrasted in the powder diffraction section are the Debye–Scherrer camera, the flat-plate camera, and the powder diffractometer. Emphasis is placed on choosing suitable film mountings and sample preparation. The relative merits of film vs. counting methods are discussed. A subsequent chapter on powder diffraction applications is excellent. Here the usual kinds of information are presented, such as indexing cubic patterns, but also included are such topics as mixtures, disorder, nonstoichiometric solids, preferred orientation, and particle size. There are lots of good examples in a self-test format, and they are often of industrial origin. There is an extensive discussion of the JCPDS Powder Diffraction File database, parts of which are reproduced and interpreted in detail. Search and match procedures are described.

The same type of format is used to describe fluorescence techniques. Both wavelength-dispersive and energy-dispersive instruments are described and actual data are presented for interpretation. Conversion tables for 2θ to λ are reproduced and utilized. Once again, the examples are outstanding and detailed. There are frank discussions on limitations and useful sections on sample preparation. Some interference effects such as absorption are mentioned. Scanning electron microscopy is an interesting inclusion in the chapter on related techniques.

Bracketing the main text is an introductory chapter and a self-test answer guide. The introductory chapter on X-rays contains the usual general information (generation of X-rays, absorption and emission, health hazards). The huge 100-page question-and-answer section does a good job of explaining the correct answer and also notes common wrong answers and why they are wrong.

In general, the language is terse with short paragraphs and frequent breaks for shaded boxes containing self-test questions [e.g., what happens when a monochromatic X-ray beam is incident on the following: (i) a stationary single crystal, (ii) a rotating crystal, (iii) a crystalline powder, (iv) powdered glass]. There are schematics and diagrams on nearly every page and they are appropriate and clearly labeled. It is easy to become accustomed to the cadence and the pace. Frequently mundane points that are important on a technical level are raised [e.g.: Is the pen out of ink? Could the presence of this element be due to contamination from perspiration?]. A recurring theme in the text's dialog with the reader is repeated drills which consider which technique is best suited for analyses of particular samples and compositions.

In its role as a study guide, the text contains peculiarities of such that make it unsuitable as a reference book: there are no references and no index, a How To Study section is included in the prologue and there is a slightly irritating congratulatory tone in the questions-and-answers section. On the other hand, I was surprised to be brought around to the conclusion that the ACOL series is probably a good idea and that this particular text is conceptually tight and consistent with those ideals. In addition to the targeted audience of commercial technicians, this book might be of interest to those of us who formally teach these topics and are sometimes in need of classroom examples.

Mary Jane Heeg, *Wayne State University*

Biological Applications of Raman Spectroscopy. Volumes 1 and 2. Edited by Thomas Spiro (Princeton University). John Wiley and Sons: New York. 1987. Volume 1: xv + 343 pp. $59.95. ISBN 0-471-81573-X. Volume 2: xi + 367 pp. $59.95. ISBN 0-471-81574-8

Over the last 20 years or so, since lasers were introduced into the laboratory, Raman spectroscopy has become a powerful tool for measuring vibrational frequencies of molecules. This has provided a wealth of structural and molecular information. Water, the essential biological medium, strongly absorbs infrared radiation but weakly scatters Raman light. Thus, Raman spectroscopy is widely used to obtain the vibrational spectra of proteins, DNA, and other biological systems. Much of the progress in this area is reviewed by various authorities in the two-volume set (soon to be three), *Biological Applications of Raman Spectroscopy*. The first volume concentrates on the conformations of biological macromolecules. Protein, nucleic acid, and lipid spectroscopy are discussed, both in isolation and in organized assemblies such as ocular lenses, viruses, and membranes. Collective vibrational modes of macromolecules are considered theoretically as there is a paucity of experimental data in this interesting but difficult area. Vibrational optical activity is also discussed in Volume 1. Resonance Raman spectroscopy is the theme of Volume 2. This effect has permitted the measurement, in exquisite detail, of the vibrational normal modes of biologically important chromophores. Specifically discussed is work on the retinal chromophores is visual pigments, purine and pyrimidine bases of nucleic acids, peptide backbone and chromophoric side chains of proteins, flavins, and resonance Raman labels (probes) of biological systems such as enzymes. The third volume will deal with heme proteins, applications to chlorophylls, and non-heme metalloproteins.

These are extremely useful books for two general types of readers. The first is the specialist in Raman spectroscopy. The technical discussion and the wealth of specific information across a wide path of biology is of great use. The second is the researcher who has an interest in a specific biological problem which might benefit from Raman spectroscopy. Raman spectroscopy is one of the many powerful physical tools developed over the past couple of decades to probe key biological issues. These books are of great use by showing how such studies have often been of use, with varying degrees of success, for various problems throughout biology.

Robert Callender, *City College of New York*

TrAC—Trends in Analytical Chemistry. Reference Edition, Volume 5: 1986. Elsevier Science Publishers: Amsterdam and New York. 1987. viii + 291 pp. Dfl. 295.00. ISBN 0-444-42772-4

This volume is a hard-bound collection of the principal content of the monthly issues of periodicals of the same name. Special attention is given to the use of computers in analytical chemistry and biotechnology. Subject and author indexes are included.