

friendly programs that can be implemented in a few hours of terminal time should look elsewhere.

ASYST consists of four modules. Module 1 consists of a graphics and statistics package. Data are input through one of several modes: by keyboard using either the self-contained editor or a special-purpose array editor, from an ASCII file using a free-format input, through the asynchronous (RS-232) port, or from one of the interface modules in real time (see below). The data can be edited, subjected to complex manipulations, and displayed graphically. Hardcopy is available on a printer or plotter using a variety of plotting formats, including arithmetic, logarithmic, and polar coordinates, as well as the usual bar graphs and pie charts. A windowing feature allows presentation of multiple graphics, e.g., decay curves and residuals, in the same plotting field.

Module 2 contains the analysis package. Complex curve-fitting functions are available. In addition, three-dimensional plotting is available, either through axonometric (perspective) or contour plots.

Module 3 is the data acquisition package. It provides software handling of the more popular analog input and output boards, including the Data Translation DT-2800 series, the Tecmar Labmaster, and the Keithley DAS 500 series. Buffered and nonbuffered I/O are supported.

Module 3 supports I/O using the General Purpose Interface Bus (IEEE-488). This software module, together with Modules 1 and 2, has become an industry standard for IEEE-488 interface communication and is often sold as a "value-added" product with digital multimeters, waveform generators, oscilloscopes, etc. A useful feature is the ability to graphically monitor analog input as it is received.

The most useful aspect of ASYST is that, as a threaded interpretive language, subroutines can be written, compiled, and executed interactively by use of keywords, which are executed whenever encountered. This allows the experienced ASYST programmer to develop programs that can be compiled and saved for use by others. Unlike FORTRAN, however, such routines are restricted to use with the original copy-protected master diskette. Experience in FORTRAN and BASIC is, unfortunately, more of a hindrance than a help, since differences from these languages can result in frustrating yet subtle errors. For instance, ASYST does not execute the last series in a DO loop. A more difficult problem is that use of arrays of variable length is almost impossible. Data are written in binary format, which makes communication with other programs difficult.

ASYST is written in a FORTH-like language. Its command structure

has more in common with reverse Polish than FORTRAN. Thus all manipulations are carried out after loading variables onto the stack, and any manipulation of a stack variable removes it from the stack. The use of stacks has the single advantage that calculations such as fast Fourier transforms become very rapid. Also, matrix manipulations can be carried out by simple statements without using DO loops. However, coding of complex functions becomes very unwieldy. For example, the function  $f(x) = x \exp(-xa)$  would be coded as follows:

```
REAL SCALAR A SCALAR X
: F(X)
  DUP X A * NEG EXP * ;
```

Since ASYST does not use statement numbers, run-time error traceback is virtually nonexistent. The manual does not even provide a complete listing of error messages, and the error messages themselves are often uninformative. Given the subtleties of some errors, this can become maddening for complex programs.

The complete ASYST package comes with five bulky loose-leaf manuals. Each manual contains a tutorial and a glossary. The tutorials are a must, but use of the indices is difficult, since topics are not extensively indexed and a single topic may be contained in two tutorials and one glossary. This reviewer generally had three or four manuals scattered over his desk whenever he attempted to use ASYST, and use of a more compact manual would have been handy. Less general information about curve-fitting and other topics and more specific information about programming subtleties would have made the manuals more generally useful.

ASYST is supplied in three copy-protected diskettes. Although the program may be copied onto a hard disk, use of the original disk is required for program startup. ASYST will run on an IBM-PC or compatible with as little as 384 kB of memory, although 640 kB is suggested for more effective use. An 8087 math coprocessor is required, as well as an IBM graphics adapter or the equivalent. The IBM Enhanced Graphics Adapter is supported as well. A plotter is a must, although only HP7475 and HP7470 plotters are supported currently.

ASYST will be useful mostly to chemists involved in real-time signal acquisition, processing, and analysis, since the plotting features are readily available in some more inexpensive forms. A disappointment for spectroscopists is the lack of a deconvolution algorithm for analysis of time-resolved spectroscopic data.

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## Book Reviews

**Methods in Enzymology. Volume 130. Enzyme Structure (Part K).** Edited by C. H. W. Hirs (University of Colorado Medical Center) and S. N. Timasheff (Brandeis University). Academic Press, Inc.: Orlando, FL. 1986. xxiii + 587 pp. \$70.00. ISBN 0-12-182030-0.

In order to have a complete understanding of how an enzyme or a protein functions and how this function is regulated, it is necessary to know its three-dimensional structure. Additionally, conformational changes occurring during protein-ligand association and the catalytic process are intrinsic to the overall mechanism. This volume details methods for evaluating protein structure in solution and methods for evaluating structural changes induced by protein binding.

The first section of 9 chapters is devoted to macromolecular assemblies and includes methods for assessing protein self-association, methods for evaluating DNA-protein interactions, and methods for determining the thermodynamic parameters for protein-ligand association. The methods described include a number of sophisticated physical techniques such as differential scanning microcalorimetry and small-angle neutron scattering. The second section of 7 chapters concentrates on optical spectroscopic methods for determining protein secondary structure, including magnetic circular dichroism and Raman and ultraviolet resonance Raman spectroscopy. In addition, a chapter on resonance Raman determination of ligand binding to metal centers is included. Conformational transitions in macromolecules constitutes the topic for the third section of 7 chapters. Within this section, the reader will find discussions of the effects of electrostatic interactions on protein conformation and conformational stability, fluorescence and circular dichroism methods for determining the kinetics of protein conformational transitions, and a calorimetric method for measuring the kinetics of lipid-phase transitions.

This volume is a valuable compilation of many recently developed, sophisticated methods for determining protein solution structure and structural transitions. In addition to their detailed presentation of the

experimental methodologies, most of the chapters include sufficient discussion of the theoretical aspects of the topic. However, many of the techniques described require sophisticated instrumentation not generally available.

Carol A. Caperelli, *Fox Chase Cancer Center*

**Methods in Enzymology. Volume 131. Enzyme Structure (Part L).** Edited by C. H. W. Hirs (University of Colorado Medical Center) and S. N. Timasheff (Brandeis University). Subedited by R. L. Baldwin (Stanford University School of Medicine). Academic Press, Inc.: Orlando, FL. 1986. xxiii + 653 pp. \$69.00. ISBN 0-12-182031-9.

This volume continues the series on methods for studying protein structure and dynamics. As with the previous volumes in this series, this volume also concentrates on physical methods.

The first section of 14 chapters deals with the subject of protein folding. It is concerned with both the dynamic and the structural aspects of this topic. A number of methods that have been developed to study the kinetics, and thermodynamics of protein folding are described, including microcalorimetry and amide proton exchange. There is also considerable discussion of methods used for the detection and characterization of folding intermediates. Some of the newer approaches to these problems that have been included in this section are the use of cryosolvents at subzero temperatures and the use of mutant proteins. The application of many of the approaches that have proved useful in studies on monomeric proteins has been attempted with oligomeric systems.

Structural dynamics and protein mobility is the subject of the second section of 10 chapters. This section is concerned with what might be termed "microscopic" aspects of protein dynamics. That is, attention is focused on small amplitude changes rather than on gross structural changes. Among the methods that are discussed are nuclear magnetic

resonance techniques, both solution and solid state; X-ray diffraction; hydrogen isotope exchange techniques; and fluorescence and Mössbauer spectroscopy.

Since it is likely that these small amplitude changes are extremely pertinent to protein stability and function and to enzymic catalysis, this volume, in particular the second section, should hold considerable interest for protein chemists and enzymologists.

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**Organic Sulfur Chemistry: Theoretical and Experimental Advances.** Edited by F. Bernardi (Universita di Bologna), I. G. Csizmadia (Lash Miller Chemical Laboratories), and A. Mangini (Universita di Bologna). Elsevier Science Publishers: Amsterdam and New York, 1985. xii + 740 pp. \$146.25. ISBN 0-444-42453-9.

This book is composed of twelve chapters covering a range of topics in organosulfur chemistry and written by internationally recognized specialists.

Chapter 1 (S. Oae) is a well-documented, historical summary detailing various bonding concepts in organosulfur chemistry. The sections of this survey are organized and discussed in terms of increased coordination number about sulfur, and this format offers the beginning researcher useful background and perspective on the development of bonding theories. It also serves as preamble to (a) concepts in hypervalency (Chapters 4 and 8), (b) stabilities of  $\alpha$ -sulfenyl, sulfinyl, and sulfonyl anions (Chapter 3), and (c) rearrangements of sulfonium ylides (Chapter 6) to mention a few. The results of electron diffraction and microwave spectroscopic studies on small organosulfur compounds are presented in Chapter 2 (I. Hargittai). Certainly, the main focus of this chapter centers on the energetics of rotational isomerism about C-S bonds with increased oxidation at the sulfur atom. Included is a short discussion on conformational preferences of the thiocarbonyl functional group as well as useful information on C-S bond lengths and C-S-C bond angles. The initial section of Chapter 3 (S. Wolfe) puts much of the past computational work on energetic preferences of carbanions adjacent to sulfur in excellent perspective. The depth of detail and discussion surrounding the possible origins of stereoelectronic effects and kinetic acidities in organosulfur compounds are particularly insightful. Chapters 4 (A. Kucsman and I. Kapovits) and 8 (R. A. Hayes and J. C. Martin) taken together represent the elements of an excellent "minisymposium" on hypervalent organosulfur chemistry. The contents of Chapter 4 detail a more general survey of numerous organosulfur compounds exhibiting sulfur-oxygen interactions. While this reviewer found the CCDB code a bit cumbersome for quickly accessing structural information, an informed view of the breath of this exciting area did emerge from the reading of this chapter. Chapter 8 is comprehensive and deals entirely with the chemistry and structural aspects of sulfuranes. This chapter brings the reader "on line" fairly quickly and provides one with a stimulating dose of the "nuts and bolts" of the sulfurane syndrome. The focus of Chapter 5 (G. Capozzi and G. Modena) is the synthesis and reactions of two classes of sulfonium salts: thiasulfonium and thiiranium/thiirenium ions. Noteworthy discussion centers on the distinction between three unique reaction paths characterizing thiiranium ions with nucleophiles. With thiirenium ions, the conclusion is that two sites of reactivity are possible and the sulfonium sulfur site is preferred over the ring carbons. Both classes of sulfonium ions are interesting although this reviewer found the former topic the most exciting with regard to potential for new research development. The following chapter (A. Fava) relates the preparation and chemistry of sulfonium ylides. This is more-or-less a general review highlighted by references to a number of synthetic applications. Chapter 7 (M. Cinquini, F. Cozzi, and F. Montanari) is intended to report the results of more recent studies on stereochemistry of chiral sulfoxides (up to mid-1983). Perhaps, out of necessity, there is overlap between this review and previous ones (ref 1 and 2) which are themselves not very old. This overlap serves to detract from the usefulness of this current review. Chapter 9 (L. Lunazzi and G. F. Pedulli) is certainly a timely review of organosulfur free radicals. The authors provide coverage on cation and anion radicals as well as pertinent discussion on "sulfur centered" radicals. The blend of ESR spectral parameters with conformational prefer-

ences makes this review particularly appealing, especially the section on sulfuranyl radicals. Chapter 10 (G. Modena, C. Paradisi, and G. Scorrano) discusses the differences in basicity and nucleophilicity between neutral sulfur and oxygen bases as well as oxyanions and thioxyanions. Several interesting conclusions emerge (i.e., inversion of basicity) from descriptions of solution and gas-phase behavior of oxygen and sulfur bases and evaluation of solvent effects employing thermodynamic cycles. Chapter 11 (I. W. J. Still) is devoted to the photochemistry of organosulfur compounds. This review is especially welcomed since the last general survey in this rapidly developing area was published in 1975. To researchers interested in this area, this review should serve as a stimulus and rich source of potentially valuable research ideas. Chapter 12 (J. Balint, R. Bogнар, and M. Rakosi) specifically addresses the chemistry and preparative techniques characterizing thioflavonoids with particular emphasis on thiocarbonyl and thioether analogues. While the focus of this chapter is a bit narrow, it does bring to light an area of research which may have new biological importance.

In summary, *Organic Sulfur Chemistry* is an excellent resource for information on some subjects in the forefront of organosulfur chemistry and is highly recommended. By and large, individual chapters are well-written and devoid of typographical errors. One or two chapters lack the elements of critical evaluation, but most succeed in bringing important subject matter to the attention of the reader.

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**Clarke's Isolation and Identification of Drugs in Pharmaceuticals, Body Fluids, and Post-mortem Material.** 2nd edition. Edited by A. C. Moffat (Home Office Forensic Science Laboratory in Huntington) et al. The Pharmaceutical Press: London (US distributor—Rittenhouse Book Distributors: 511 Fehely Drive, King of Prussia, PA 19406). 1986. xix + 1223 pp. \$132.00. ISBN 0-86369-166-5.

This large-scale compendium of analytical and toxicological information on over 1300 drugs, methods, and reagents is an essential reference for clinical chemists, clinical toxicologists, analytical chemists, forensic chemists, forensic toxicologists, drug researchers, and students who need to identify drugs in pharmaceuticals or body fluids and tissues. As in the first edition of this classic, the largest section describes the analysis and toxicology of individual compounds. This includes infrared, ultraviolet, visible, and fluorescence data and spectra; molecular weights, formulae, and structures; color tests, thin-layer (TLC), gas (GC), and high-pressure liquid (HPLC) chromatographic data; immunoassays; and principal mass spectral peaks as well as biological disposition, dose, therapeutic concentrations, toxicity, half-life, volume of distribution, distribution in blood, clearance, and protein binding on many substances. New drugs have been added in place of some of the more esoteric ones. Spectra appear conveniently with other specific drug data, a significant improvement over the appended spectra in the first edition. In addition, the spectra are larger and easier to read due, in part, to a slightly larger page format.

Of the remaining parts, the first consists of 18 chapters by 23 British experts on various topics related to drug analysis. Completely rewritten, updated chapters on gas chromatography, infrared spectrophotometry, and color tests supplement new chapters on other methods, skills, approaches, and applications such as hospital toxicology, drug abuse screening, pesticides, drug abuse in sports, inorganics, HPLC, and immunoassays. Chapters on paper chromatography and microcrystal tests have been deleted, shifting the book's apparent aim toward more sophisticated analysts. Additional indexes of analytical data comprise the third part. Ascending molecular weights, melting points,  $R_f$  values for TLC systems, retention index for GC systems,  $k'$  values for HPLC, UV maxima, principal IR peaks, and principal mass spectral peaks ( $m/z$ ) form a practical subreference to the 18 chapters in Part 1. The fourth, and shortest, section lists recipes for color test and TLC visualization reagents as well as commercial sources (mostly British) for some of the test materials described. Finally, a general index allows the user to find virtually any subject contained in this comprehensive work.

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