



Figure 4. Another view of our model with perspective turned to maximum and magnification set to 200% (300% is the maximum magnification allowed). The drawing was reduced to 50% after pasting into Word.

minimization. The only minimizer in MicroChem is the ring-creating facility in BuildMol. TwistMol does, however, calculate steric and electrostatic strain energy for any conformation input into the application. The Del Re method is used to estimate partial charges on the atoms, or you can supply your own charges. TwistMol *does not* allow any changes of bond lengths or angles from within the application.

What TwistMol does allow, however, is a "fixed valence" molecular mechanics calculation, where energies are computed for rotamers generated by rotation about single bonds. Thus, one may select a bond, an arc (e.g. from 0° to 180°), and an increment (e.g. 10°), and let TwistMol generate a family of rotamers, and calculate the strain energy for each. After completion of the calculation, the lowest energy conformation is displayed, and all of the data generated in the calculation are stored in a text file. As many as 10 bonds may be selected in this process to generate an array of conformations that are screened in one batch process. Scanning rotamers about one bond is fairly quick (a 0°–180° scan in 10° increments on one of the Ar–Ar single bonds in our model took a little over 1 min on the Mac II). However, naturally the more bonds selected, the longer the process takes. Patience here is necessary. In the manual, it is stated that torsional parameters will be included in future versions, but the version reviewed did not include any torsional strain in the calculations.

While clearly very interesting, I am not sure how useful TwistMol will really be. The fixed valence approach for scanning rotamers only provides a very approximate picture of the conformational surface of a molecule. For example, scanning *n*-butane in 10° increments about the C2–C3 bond gave the anti conformation as the minimum. However, the conformation with a dihedral angle of 90° was only 0.01 kcal/mol higher in energy according to the calculation. For the axial and equatorial methylcyclohexanes, even with a scan in 10° increments about the C1–methyl bond, the axial conformer came out more than 5 kcal/mol above the equatorial conformer.

Upon completion of a scan, TwistMol puts the data obtained from the scan in a text file. Opening this file with a word processor allows a quick perusal of the conformations and strain energies obtained in the scan. Unfortunately, due to the way MicroChem delimits columns and presents the data, I was not able to devise a simple way to get the data into a spreadsheet or plotting program to plot the surface. The manual states that future versions will include a plotting facility.

Finally, TwistMol includes a utility affording some control over ring conformations. Thus, starting with chair cyclohexane, selecting the "pucker" command, and then clicking on one of the carbons of the chair affords a boat. I cannot comment on the general availability of this option, however, since with any decalins, every time I tried the pucker command, a message appeared stating something to the effect that MicroChem could not change the pucker of that carbon. As described above, InputMol allows some control of ring conformation with the stereochemistry option.

Overall, the MicroChem Organic Module provided some very useful tools. I was able to easily input crystal coordinates into my Mac and examine a 3-D model of the crystal structure in stereo. This, with the Newman projection option, made construction of a Dreiding model of the structure trivial. Of course, the same features are available on other

Mac applications at a lower cost (e.g. Ball&Stick). However, with MicroChem I could then modify my structure by rotating about acyclic bonds, perform some simple energy calculations, and get very nice looking presentation graphics for inclusion in a proposal or publication.

That is the good news. Unfortunately, I found the limitations and quirks of the program to be bothersome. While the limitation on the number of atoms (500) did not present a problem for me, I was frustrated by the lack of support for displaying more than one molecule on the benchtop at one time. Thus, it is not possible to create complexes or perform even rudimentary modelling of "docking" processes. For presentation graphics, this problem can be circumvented somewhat by using a vector drawing program (e.g. MacDraw II). Since the models transfer as vector images, it is quite simple to "eclipse" parts of one molecule with another to create non-covalent complexes.

Finally, in my view MicroChem affords a very poor implementation of the Mac interface. Most glaringly, the method used for rotations was actually *worse* than the typical IBM-style command-oriented approach. In order to rotate about a given axis or bond, a command (e.g. Rotate X) is selected from a menu. This brings up a dialog box at the bottom of the screen with a scroll bar and number indicating the rotation in degrees. Clicking on the arrows changes the rotation in 1° increments, but on the Mac II scrolling is so fast it was almost impossible to stop at a specific number. Clicking on either side of the box in the scroll bar changed the number in 5° increments. After hitting the value of the rotation I wanted, it was necessary to then select "Redraw" from a menu to obtain the rotated structure.

Incredibly, while rotation is possible in all applications but BuildMol, it is implemented in at least three different ways. The Rotate and Redraw commands sometimes appear in the same menu, and sometimes in different menus. A partial saving grace is that *every* command in every application has a Command-key equivalent. In all modules supporting rotation, Command-j, Command-k, and Command-l do not open the dialog box, but rather perform a 30° rotation about the X, Y, and Z axes, respectively. Thus it is possible to be looking at a 3-D stereoview and rotate from the keyboard somewhat interactively. Holding the Command-key down continues the rotation, a bit more slowly than the animation facility in DisplayMol, but similar. This Command-key rotation facility, in my view, saves the program from being unusable, though it would be great to be able to change the default rotation increment from 30°, which is a bit too large.

Naturally, it is often desirable to reverse the direction of the rotations. According to the manual, this is done in a standard Mac fashion by using the Option-Command-key combination. However, in my version of the program, this approach did not work. Instead, Shift-Command-key reversed the direction of the rotation—but every time! Thus, in order to reverse rotation directions, it was necessary to use the Shift key *only once*. Command-key strokes then continued rotating in that direction until the Shift key was used again. Another example of deviation from the standard Mac interface is the method of stopping a minimization in BuildMol. The standard Mac method would be Command-period. In MicroChem, one clicks the cursor in a bar on the right of the screen, where the scroll bar would normally be, to stop the calculation.

This may sound like nit-picking. But, Mac users expect an intuitive, innovative interface. To find such a cumbersome approach to 3-D rotation on the Mac was very disappointing. Also, the version I reviewed seemed loaded with glitches and bugs. For example, often rotation of space filling models would show nonsense at certain views. This was even true for benzene, where the carbons seemed to jump out of the ring in some views. In AssembleMol, when using the "invert" command to change axial to equatorial substituents, choosing "Save As" from the "File" menu *overwrites* the original file on disk, while choosing "save" brings up a dialog box for renaming the file. Be careful of this one! Finally, on the Mac II under MultiFinder, a system crash was guaranteed during a long session, though the time between crashes was long enough that useful work could certainly be accomplished.

In summary, given that MicroChem is really the only game in town right now, and that upgrades are promised in the future, I feel that many chemists equipped with Macs will find the program very useful. Also, the manual advertises a Mac II-specific version called MicroChem/XP, which takes advantage of the 68881 coprocessor and announces a color version coming soon. With some improvements in the interface, and true minimization capabilities, MicroChem could become a truly outstanding tool for professional chemists.

David M. Walba, *University of Colorado*

Book Reviews

Lecture Notes in Chemistry. Volume 40. Time-Dependent Reactivity of Species in Condensed Media. By A. Plonka (Technical University, Łódź). Springer-Verlag: Berlin, Heidelberg, and New York. 1986. iii + 151 pp. \$22.00. ISBN 3-540-16796-X; ISBN 0-387-16796-X.

There is increasing interest in physical relaxation processes and unimolecular or single-step chemical reactions that do not conform to the single exponential decay law expected for first-order kinetics. This book is addressed primarily to chemists who are interested in the analysis and interpretation of such anomalous reaction patterns in systems as diverse as glassy matrices, polycrystalline ice, bulk polymers, and micellar solutions. A unifying feature is that most of the experimental work surveyed in the book deals specifically with the reactions of radicals and radical ions in these systems.

The analysis of time-dependent reactivity can proceed along several different lines, and the author's approach is premised on the use of one particular form of time-dependent rate constant as given by the equation, $k(t) = Bt^{\alpha-1}$, where B and α are empirical constants with α being in the range from 1 to 0. Perhaps the simplest physical meaning that can be attached to this equation is that it reflects a distribution of activation energies, the smaller values of k at longer times corresponding to larger activation energies for the reaction. However, the author considers that no unique physical mechanism is likely to be generally responsible for dispersive kinetics of this type, and the possible molecular origins of the reactivity distributions are discussed with the aid of mathematical formalisms in the final chapter. This cautious approach is certainly justified by the variety and complexity of the systems under consideration.

To the extent that the author does invoke a general physical model to describe the phenomenological kinetics, it is that of nonexponential relaxation or the emergence of a "waiting-time distribution" as a necessary prelude to obtaining the critical configuration for reaction. For example, trapped hydrogen atoms in low-temperature aqueous glasses are considered to be liberated for reaction by trap destruction through matrix relaxation. In fact, the major theme of the book is the author's emphasis on the striking parallel between nonexponential decays in chemical reactions and in relaxation processes, as illustrated by the successful adoption of the Kohlrausch relaxation function for the analysis of some of these time-dependent reactivity patterns.

There are other ways of accounting for nonexponential kinetics, but these are not developed in detail. One such approach is simply to regard the reactivity pattern as originating from a distribution of reaction sites, the rate at each site now being an intrinsic function of the particular site geometry that remains unaffected by relaxation or cooperative processes. Although not mentioned in the book, this model has been applied [*Faraday Discuss. Chem. Soc.* **1984**, *78*, 175; *Acc. Chem. Res.* **1986**, *19*, 238] to describe the composite first-order kinetics of hydrogen-atom abstraction by alkyl radicals in alcohol and alkane glasses. In this case the physical basis for the model is provided by quantum-mechanical tunneling [Bell, R. P. *The Tunnel Effect in Chemistry*; Chapman and Hall: London, 1980; Chapter 5, p 106], the reaction rate depending on the distance of hydrogen transfer which naturally varies from site to site in an inhomogeneous medium.

Few scientific errors were noted, but unfortunately some of the lengthy discussion in Chapter 2 on alkyl radical decay in organic matrices (pp 52-60) perpetuates some original interpretations of the data that have long been superseded. Specifically, it was assumed in some of the early work that alkyl radicals decayed by geminate recombination with their halide ion or other partners, and the effect of matrix deuteration on the rate was attributed to collective effects associated with solvent configurational requirements for this recombination. However, it has been shown by ESR spectroscopy [*J. Am. Chem. Soc.* **1972**, *94*, 7633] that the correct mechanism for alkyl radical decay in these systems is by hydrogen-atom abstraction from the solvent, the very large effect of solvent deuteration on the rate at low temperatures being properly interpreted in terms of the difference between H and D tunneling. This example illustrates the importance of having a physical and molecular model of the reaction mechanism that can be independently verified, just as in other branches of chemical dynamics. Conversely, it shows some of the pitfalls associated with models that can only subscribe to a formal mathematical explanation of complex kinetic data. Of course, the microscopic origin of multiexponential decays is not always readily amenable to direct characterization, a point that is touched upon repeatedly in the book.

In summary, these timely lecture notes constitute a veritable mine of information on the condensed-phase reactions of free radicals showing dispersive kinetics, and Dr. Plonka is to be congratulated on bringing so much of this diverse material together in a readily assimilable form. Hopefully, this monograph will stimulate additional work designed to probe the more fundamental aspects of this subject.

Ffrancon Williams, *University of Tennessee, Knoxville*

Industrial Aromatic Chemistry: Raw Materials, Processes, Products. By H.-G. Franck and J. W. Stadelhofer (Rütgerswerke, Frankfurt, FRG). Springer-Verlag: Berlin and New York. 1987. xiv + 486 pp. \$79.00. ISBN 3-540-18940-8 and 0-387-18940-8.

This book is packed with considerable information on aromatic hydrocarbons, including a historical review (Chapter 1), nature of aromatic structure and basic chemistry (Chapter 2), and feedstocks used for producing various aromatics (Chapter 3). The production of aromatics is described in the latter chapter (of 70 pages) from coal, crude oil, pyrolysis processes, alcohols, and renewable materials; obviously the space allotted to each process is highly limited and few details are reported.

Chapters 4, 5, 6, and 7 discuss the production of benzene, toluene, and xylenes and the products obtained from each. In recovering high-purity aromatics, several separation techniques are discussed, including ordinary distillation, extractive distillation, azeotropic distillation, and crystallization. Dealkylation, disproportionation, and isomerization reactions are often required to obtain the preferred aromatic. In many cases, alternate methods of producing a desired product are outlined; the advantages and disadvantages of these alternate processes are reported to only a very limited extent at best. In several cases, modern processes of importance have not been included; examples are the ethylbenzene process of Monsanto/Lummus, aniline processes, and aromatic nitration processes. Many products that can be obtained are, however, succinctly mentioned. In the case of benzene, a *partial list* of obtainable products includes ethylbenzene, styrene, cumene, phenol, Bisphenol A, nitrobenzene, aniline, cyclohexylamine, maleic anhydride, chlorinated benzenes, and hexachlorocyclohexane.

Chapters 8-14 discuss the production and use of polyalkylated benzenes, naphthalene, alkylnaphthalenes, anthracene, other polynuclear aromatics, mixtures of condensed aromatics, and aromatic heterocyclics. The toxicology and environmental aspects of aromatics is considered in Chapter 15.

Although many important aspects and several modern processes have been omitted, the book will be a welcome source of general information.

Lyle F. Albright, *Purdue University*

Advances in Mass Spectrometry 1985. Part A and Part B. Edited by J. F. J. Todd (University of Kent). John Wiley & Sons: Chichester and New York. Part A: 1985. xxx + 565 pp. Part B: 1986. xliii + 1091 pp. \$370.00. ISBN 0471-90831-2.

These two volumes contain the papers presented at the 10th International Mass Spectrometry Conference, which was held in Swansea, UK, in September 1985. Part A includes the full texts of the plenary and keynote lectures, while Part B contains the two-page extended abstracts of the contributed papers.

The opening address by J. I. G. Cadogan is an interesting and informative history of mass spectrometry and the international conferences. The plenary lectures were the following: Applications of Mass Spectrometry in Biology, Pharmacology, and Medicine by E. C. Horning; Mechanistic Aspects of Organic Mass Spectrometry as Exemplified by the Experimental/Theoretical Study of Ionized Keto/Enol Tautomers by H. Schwartz; Instrumentation in Mass Spectrometry by J. F. J. Todd; Developments in the Theory of Mass Spectrometry by J. C. Lorquet, C. Barbier, and B. Leyh-Nihant; and The Physical Chemistry of Ion Reactions. Clusters and Macromolecules by P. J. Derrick.

There were 26 keynote lectures covering a wide variety of topics. A representative group includes the following: GC/MS Employed with Chemical Ionization Sources for Studies of Positive and Negative Ions by A. P. Bruins; Mass Spectrometric Studies of Halley's Comet by J. Kissel; Mass Spectrometric Studies at High Temperature by J. Drowart; Analysis of Inorganic Solids and Solutions by Plasma Source Mass Spectrometry by A. L. Gray; Ab initio Calculations of Positive Ions by P. von R. Schleyer; Low Energy Ion-Molecule Reactions by K. R. Jennings; Photodissociation of Ions by K. Levsen; Cluster Ions by T. D. Märk; Tandem Mass Spectrometry by F. W. McLafferty; and Collisional

Processes of Negative Ions: Analytical and Mechanistic Aspects by J. H. Bowie.

The abstracts of the more than 500 contributed papers are published in Part B. These abstracts are grouped into the following 15 different subject areas: liquid chromatography/mass spectrometry, gas chromatography/mass spectrometry, ion structures and mechanisms, instrumentation and novel techniques, laser-induced ionization and excitation, high-temperature studies and inorganic analysis, isotopic measurements, cluster ions, physical and theoretical, data processing, biomedical applications, pyrolysis mass spectrometry, new spectra, tandem mass spectrometry, and desorption ionization.

With the total of nearly 600 papers or abstracts contained in the two volumes, this publication is a comprehensive account of the methods and applications of mass spectrometry. These books should be an excellent reference source for anyone interested in mass spectrometry.

Lynford L. Ames, *New Mexico State University*

Modern Techniques of Surface Science. By D. P. Woodruff and T. A. Delchar (University of Warwick). Cambridge University Press: Cambridge. xi + 453 pp. \$24.95 (paperback). ISBN 0-521-35719-5.

During the past decade, the field of surface science has been growing extremely rapidly. This growth has been characterized in part by a proliferation of analytical techniques, each with its own three- to six-letter acronym. The need for many experimental approaches has resulted from the fact that no one of them completely solves a given problem in surface science. Thus, surface scientists must be keenly aware of the strengths and weaknesses of all the techniques. Over the years, a number of monographs devoted to individual surface analysis methods have appeared. Recently, Woodruff and Delchar have written a comprehensive volume describing all the major analytical techniques that are currently used in ultra-high vacuum (UHV) surface studies. Clearly, such a book is a welcome addition to the field.

The topics the authors cover include surface crystallography and diffraction (LEED, RHEED); electron spectroscopies (XPS, EXAFS, SEXAFS, AES, ILS, UPS); vibrational spectroscopies (IRAS, HREELS); incident ion techniques (INS, ISS, Rutherford scattering, SIMS); desorption spectroscopies (TDP); high-field techniques (FEM, FIM); work function techniques; and atomic and molecular beam techniques. The only obvious omission, which is noted by the authors, is scanning tunneling microscopy (STM). STM is very new and was only beginning to be widely applied as the book was being written.

For each technique, Woodruff and Delchar discuss the basic physics of the processes involved, as well as the theoretical basis of the data interpretation. They also describe in some detail the experimental apparatus required to perform the techniques. Finally, the authors outline a number of applications and provide appropriate figures taken from original references.

This book is an excellent reference and source of general learning material for practitioners and graduate students in surface science. It covers all the major topics in sufficient detail that one need not read further if only a general understanding is required. However, for each topic, a variety of references are given, so that further detailed information may be easily obtained if desired.

Barbara J. Garrison, *The Pennsylvania State University*

Major Chemical Hazards. Ellis Horwood Series in Chemical Engineering. By V. C. Marshall. Halsted Press, a division of John Wiley and Sons: Chichester. 1987. xv + 587 pp. \$105.00. ISBN 0-85312-969-X.

The treatment of chemical hazards in a comprehensive publication, which includes a complete description of chemical hazards and related case histories, was not available until now. V. C. Marshall, a safety professional and chemical engineer, has produced such a book.

With our society at a seemingly high level of chemophobia, this text has put into perspective for the readers the real hazards associated with chemicals. The author describes the hazards and the level of harm but goes further to summarize the potential and consequences of realizing the harm. He accounts for the control measurements needed to minimize the possibility of injury and finally reports on the methods that could reduce the consequences. In summary, he takes the traditional approach of recognition, evaluation, and control when dealing with hazardous substances.

The uniqueness of the book is that forty actual case studies, not scenarios, are used throughout the book to illustrate the specific chemical hazards. Some of these case studies include Cleveland, Ohio (liquefied natural gas spill), Texas City (ammonium nitrate explosion), Mexico City (liquefied propane gas explosions); a number of rarified explosions like Westwego, Louisiana, and Galveston, Texas (grain dust explosions), Staten Island, New York, and Sheffield, England (confined space explosions); Mississauga, Toronto, Canada (chlorine, train derailment), Bhopal, India (methyl isocyanate release).

The specific hazards of fire/explosion and toxic releases are outlined and are described in detailed technical terms. A particularly good chapter deals with the quantitation of these hazards. Here a review of vapor-cloud formation and dispersal is presented. Also included in the text are suggestions for safety training and the role of hazardous chemical research.

I find this publication to be one of the best of its kind on the market and Dr. Marshall must be commended for his efforts. It is contemporary with over forty case studies evaluated in light of proper technical thought. The material presented is at a level that is appropriate for safety professionals, chemists and chemical engineers, industrial hygienists, and students of chemistry and chemical engineering.

Thomas J. Haas, *United States Coast Guard Academy*

Nuclear Magnetic Resonance—Basic Principles. By Atta-ur-Rahman (University of Karachi). Springer-Verlag: New York, 1986. ix + 358 pp. \$59.00. ISBN 0-387-96243-3.

This book aims to give a comprehensive introduction to 1-D and 2-D ¹H and ¹³C solution NMR without too much mathematics. It is intended for chemists, biochemists, and other users of NMR. It touches briefly and qualitatively on most of the principles and practices germane to the applications of NMR it addresses. It goes into considerably more detail when covering the details of spectral interpretation.

The first two chapters cover the basics of ¹H NMR, first chemical shift and then spin-spin coupling. The latter is covered in some detail. The third chapter deals with experimental procedures: FT methods, simple pulse sequences, and relaxation. It lets the latter topic lead the chapter into consideration of the NOE and dynamic effects. The fourth chapter deals with ¹³C NMR. It is briefer than the two chapters on ¹H NMR, but it accomplishes this by the extensive and effective use of tables. The fourth chapter also manages to include a bit on solid-state ¹³C NMR and magnetic resonance imaging, doubtless for cultural purposes. The fifth chapter (fully one-third of the text) discusses 2-D methods. It presents numerous pulse sequences, energy level diagrams, spin vector plots, and sample spectra. The text proper is followed by a collection of problems concerned with the interpretation of ¹H and ¹³C spectra (with solutions).

This book has many useful features, e.g., extensive tables, detailed qualitative explanations based on examples, and the problems. NMR theory is less satisfactory, because it is so qualitative; to the audience at which the book is directed the level may be the preferred one. The weakest parts of the book are the figures. First, many of them are inadequately referenced. A figure caption that merely says: "Reprinted with permission from *J. Am. Chem. Soc.*, Copyright 1979, The American Chemical Society," when the text provides no further information about the source, deprives the reader who would pursue the subject. Second, some of the figures are clearly freehand drawings of the sort one might put up on a chalkboard. This lends a certain charm; but, in a few, the point to be made is obscured by distracting inaccuracies.

E. O. Stejskal, *North Carolina State University, Raleigh*

Structure and Bonding. Volume 67. Coordination Compounds: Synthesis and Medicinal Application. With contributions by R. A. Bulman (National Radiological Protection Board, Didcot, U.K.), A. M. J. Fichtinger-Schepman (Medical Biological Laboratory, Rijswijk), R. Krause (University of Connecticut), and J. Reedijk, A. T. van Oosterom, and P. van de Putte (Leiden University). Springer-Verlag: Heidelberg and New York. 1987. 150 pp. \$60.00. ISBN 3-540-17881-3.

This volume contains three review articles with the general description Coordination Compounds; Synthesis and Medical Applications. The first of these is a discussion of the Synthesis of Ruthenium Complexes of Aromatic Chelating Heterocycles: Towards the Design of Luminescent Compounds. An orderly sequence of subtopics gives the synthesis of potentially luminescent Ru(II) species, with a nice discussion of the merits of use of each of the available precursors, and the best procedures are described in some detail. The discussion includes tables of structures for each of the commonly-used acronyms for the many variations in ligand type based on pyridine and the other simple heterocycles. Models for the excited state of these species are reviewed, with special consideration given to the effects of molecular structure on excited-state behavior. A very complete set of tables are included which summarize the properties displayed by emitting complexes, such as quantum yield and radiative lifetime. Variations caused by changes in ligand type, ligand substitution, and solvent system are discussed. This review contains 274, mostly quite recent, references to the field, including numerous contributions from the laboratories of F. Bottomley, D. J. Cole-Hamilton, Glenn Crosby, Keith DeArmond, Jim Demas, Harry Goodwin, M.-A. Haga, John Kelly, A. B. P. Lever, A. Ludi, Tom Meyer, and A. v. Zelewsky.

The second review, authored by J. Reedijk, A. M. J. Fichtinger-

Schepman, A. T. van Oosterom, and P. van de Putte, is entitled "Platinum Amine Coordination Compounds as Anti-Tumor Drugs. Molecular Aspects of the Mechanisms of Action". It is a thorough overview of the history, use, mode of action, and side-effects of "cisplatin" and its close analogues and anticancer agents. Attention is given to the relationship between observed biological activity and the structure of the complex, with special emphasis on the nature of the ligands coordinated to platinum. The primary biological event, which appears to involve disruption of nucleic acid stacking by coordination of platinum to basic nitrogen sites, especially at N-7 atoms of guanine residues, is discussed in great detail. A host of studies of "cisplatin"-type interactions with mono-, di-, and tri-, and larger nucleotides are cited, giving rather convincing evidence of the chelation of the *cis*-Pt(NH₃)₂ units to these fragments as the major deactivation pathway. In vitro and in vivo studies are compared, showing similar coordination to DNA, but not to RNA systems. This review, which contains 163 recent references, concludes with a compendium of unanswered questions about the activity of "cisplatin" and its analogues, providing starting points for experienced or new workers in this very important area. The multidisciplinary character of "cisplatin" research should make this article especially interesting to chemists, biologists, pharmacologists, medical oncologists, and other researchers.

The final review, authored by R. A. Bulman, is a very extensive overview entitled "The Chemistry of Chelating Agents in Medical Sciences". A good introduction to the field is given, followed by a compilation of the manner in which chelating agents find current medical utilization, including toxic ion mobilization, essential element mobilization and regulation, non-invasive diagnostic medicine, anti-inflammatory agents, and antineoplastic, antiviral, antimicrobial, and antiparasitic agents. The myriad of such ligands prepared and investigated for these uses are nicely classified, with examples of hard- and soft-bases, chelating ligands of a wide range of denticity, cyclic systems, those of microbial or fungal origins, and other species. Some of the newer uses of chelates are discussed, including their capacity to carry either γ -emitting or paramagnetic metal ions to specific body regions. The development of NMR techniques involving metal isotopes has led to additional diagnostic medical tools, and work in this area is covered as well. A significant portion of the review is devoted to the directions taken in synthesis of new chelating agents containing a number of different functional groups. The review contains a rather complete table of the pertinent acronyms encountered in this area and cites 333 modern references. It should be a welcome addition to the libraries of all medical colleges and pharmacological research teams. The relatively low cost, and the thoroughness of each of the three reviews, should make this text a valued addition to the others in the Structure and Bonding Series.

David Allan Owen, Murray State University

Two-dimensional NMR Spectroscopy: Applications for Chemists and Biochemists. Edited by William R. Croasmun and Robert M. K. Carlson. VCH Publishers: New York and Weinheim. 1987. xx + 511 pp. \$95.00. ISBN 0-89573-308-0.

This book is Volume 9 in the series *Methods in Stereochemical Analysis*. It consists of nine chapters, all written by researchers with hands-on experience with the modern two-dimensional (2D) NMR techniques. The aim of the book is to promote a wider use of 2D NMR spectroscopy in the solution of stereochemical and more general chemical problems. To this extent, Chapters 4 and 9 discuss the use of 2D NMR for a variety of different classes of chemical compounds.

The first two chapters, by George Gray and William Hull, are intended to provide some simple theory of two-dimensional NMR, and more importantly, it contains many "insider tips" on how to record optimum quality spectra. I find the advice given generally sound and it should be useful not only to the novice but also to the regular user of advanced high-resolution NMR techniques. Hull's chapter (165 pp) is partly written in Bruker language, which may make it harder to read for the non-Bruker user. Alternatively, for Bruker users this chapter alone is worth spending \$95. The third chapter discusses what kind of experiments to use for what kinds of problems, information that is largely duplicated in the following chapters by authors that discuss their own chemical applications.

Chapter 4, by Kessler and co-workers, illustrates the use of 2D NMR experiments for obtaining complete ¹H, ¹³C, ¹⁵N assignments of the peptide, cyclosporin A. The spectra shown are beautiful examples of the power of 2D NMR in the study of peptides. However, it should be noted that for less well behaved peptides, without the exceptionally high solubility of cyclosporin A and without an organic solvent, many of the approaches shown may become too difficult for routine use. Chapter 5, by David Kearns, discusses the use of 1D and 2D NOE experiments for the study of DNA conformation.

Chapter 6, by Janusz Dabrowski, discusses the application of 2D

NMR to complex carbohydrates and polysaccharides. Some of the ancient SECSY representations should not be present in a 1987 book, but in general, the chapter gives a good overview of modern carbohydrate NMR without going into the most sophisticated experimental techniques. Chapter 7, written by the editors, discusses the use of NMR for steroid analysis, and in Chapter 8, Peter Rinaldi illustrates the use of 2D NMR for structure determination of a typical organic product. Finally, in Chapter 9, Gary Martin discusses a number of applications to organic products with emphasis on the study of polycyclic aromatic compounds.

All authors are experts in their areas of research and the book contains a set of beautiful illustrations to a large variety of compounds. As often is the case in a multi-author volume such as the present one, there is a large amount of duplication between the various chapters. At least several dozen very similar looking COSY spectra are spread throughout the book, although the question on how to measure a coupling constant from such a spectrum is answered differently by different authors. Treatment of a number of unillustrated specialized 2D techniques in the earlier chapters could have been cut by the editors. Overall, however, the book is certainly interesting and nonmathematical, and it should be stimulating to those chemists who are still restricting themselves to the use of more conventional one-dimensional experiments.

Ad Bax, National Institutes of Health

Neuromethods. Volume 9. The Neuronal Microenvironment. Edited by A. A. Boulton, G. B. Baker, and W. Walz (Universities of Saskatchewan and Alberta). Humana Press: Clifton, NJ. 1988. xxvi + 732 pp. \$94.50. ISBN 0-89692-115-2.

The detailed manner in which many chemical and physical measurements are performed by neuroscientists is frequently somewhat obscure to chemists interested in the field. The series of monographs by Boulton, Baker, and selected co-authors admirably removes a great deal of this obscurity by providing in-depth accounts of the methodology which inform the reader how to do it, the advantages and disadvantages, the necessary practical considerations, the alternatives available, and how the data obtained might be applicable to neurobiological questions at hand. The current volume in this series is yet another excellent addition which will be of considerable help to the novice as well as offering unique insights to the expert. Its primary focus is upon extracellular space, which represents approximately 20% of total mammalian brain volume. This region has only been recognized as having a substantial effect upon neuronal excitation processes in the past decade. The individual chapters cover topics generally familiar to the chemist (potentiometry, voltammetry, and spectroscopy) as well as some more recent procedures (computer tomography and NMR) applied to such investigations. Both in vivo and in vitro (brain slices, cell cultures) preparations are considered. The chapter by Nicholson and Rice on ion-selective and voltammetric micro-sensors is particularly comprehensive and well written. There are two shortcomings in this reviewer's opinion. First, the chapter covering ultrastructural methods is too brief; it does not contain the detail consistent with the remainder of the book. Second, there is no chapter on the microdialysis technique. This technique is rapidly becoming one of, if not the most popular for the investigation of extraneuronal space. While the chemist will frequently encounter familiar concepts (pH, ion activities, etc.) in this volume, s/he will also quickly realize the difficulties associated with applying these established concepts to the non-homogeneous, non-equilibrium, barrier-bounded biological system in which the neuron is found.

C. LeRoy Blank, University of Oklahoma

Oxygen Complexes and Oxygen Activation by Transition Metals. Edited by A. E. Martell and D. T. Sawyer (Texas A&M University). Plenum Press: New York. 1988. ix + 341 pp. \$62.50. ISBN 0-306-42789-3.

This monograph reports the proceedings of the fifth IUCCP (Industry-University Cooperative Chemistry Program) Symposium on Oxygen Complexes and Oxygen Activation by Metal Complexes, held at Texas A&M University on March 23-26, 1987. It includes 18 invited papers by experts in the field from both academic and industrial laboratories and 20 abstracts of submitted posters. Comments and summary statements are provided by F. Basolo and D. T. Sawyer, and a subject index is included. In general, the papers are succinct summaries of research from the authors' laboratories rather than lengthy reviews. In all cases, key references are provided to guide the reader to more specific information.

The first section of the book contains seven papers on dioxygen binding by transition metals. It begins with a discussion of molecular orbitals and bonding of O₂ to metals and is followed by papers on both metallo-proteins which act as O₂ carriers and their synthetic models, with an emphasis on physical characterization of metal-oxo and metal-dioxygen compounds. A second section includes 11 papers on activation of dioxygen by transition-metal complexes. Here, the discussion also includes examples from both biological and model systems. Synthetic cobalt,

copper, vanadium, iron, and palladium catalysts for oxidation are presented which include studies in homogeneous solutions as well as on surfaces or in zeolites. A balance of experimental results of oxidation reactions and mechanistic interpretation is provided.

This book incorporates an unusual number of contributions from industrial laboratories (7 out of 18 invited papers) which affords the reader an additional perspective on aspects of O₂ binding and catalysis of oxidation important to industry. Although it does not give comprehensive coverage of the field of metal-dioxygen chemistry, this monograph furnishes an excellent summary of many key areas and could be a starting point for those just entering the field.

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Topics in Current Chemistry. Volume 142. Electrochemistry I. Edited by E. Steckhan. Springer-Verlag: Berlin, Heidelberg, and New York. 1987. 195 pp. \$75.00. ISBN 0-387-17871-6.

This volume contains five reviews of topics in organic electrochemistry written by recognized authorities. All the reviews emphasize research in the last decade or so and contain a healthy dose of electrochemical mechanistic detail. Since the work of European and Asian researchers dominates recent developments in organic electrochemistry (with notable exceptions, e.g., the contributions of the late M. M. Baizer and contributions in photoelectrosynthesis described by M. A. Fox), American researchers contemplating an electrochemical synthetic procedure may find this volume to be informative.

E Steckhan thoroughly reviews "Organic Syntheses with Electrochemically Regenerable Redox Systems", covering both inorganic and organic mediators and many examples (327 references). In the chapter by M. A. Fox, "Selective Formation of Organic Compounds by Photoelectrosynthesis", a qualitative description of the physical chemical processes operative at illuminated semiconductors is given. She considers the roles of the energy levels, the band gap potential, current density, and surface conditions as they effect selectivity for photoelectrochemical transformations. Examples given include oxidations, reductions, cycloadditions, retrocycloadditions, and geometrical isomerizations (194 references). The chapter by H.-J. Schäfer on "Oxidation of Organic Compounds at the Nickel Hydroxide Electrode" has a practical bent. Electrolysis conditions and yields are given, and comparisons are made with alternative synthetic methods, e.g., the use of nickel peroxide (91 references). The final two contributions are complementary: "Electrogenerated Bases" by J. H. P. Utley (58 references) and "The Chemistry of Electrogenerated Acids" by K. Uneyama (52 references). Both are well organized essays that bring together recent work in electrochemistry. By way of examples, these authors show how the electrolyte and solvent can influence the acid-base chemistry of the reactions coupled to the charge-transfer steps in electrosynthetic procedures.

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Photoelectrochemical Solar Cells. Edited by K. S. V. Santhanam (Tata Institute of Fundamental Research) and M. Sharon (Indian Institute of Technology, Bombay). Elsevier: Amsterdam. 1988. xii + 372 pp. \$144.75. ISBN 0-444-42910-7.

This volume provides an introduction to semiconductor electrochemistry summarized from an international training workshop conducted by UNESCO in 1986 at the Indian Institute of Technology in Bombay. It takes the reader from a very elementary level to a stage where many of the important problems in semiconductor electrochemistry can at least be appreciated. It would appeal both to chemists and solid-state physicists who have research interests in this important area of electrochemistry and material science.

After an overview chapter by the editor, an excellent discussion of the physics of semiconductors and small pn junctions by S. Roy Morrison ensues. Morrison's chapter builds from an elementary consideration of the band model of semiconductors to describe the construction of junctions and transistors that can be characterized by electronic or optical effects. The importance of interfacial catalysis and dislocations and surface states is clearly presented.

Techniques for characterization of semiconductors are then considered. The chapter by Micha Tomkiewicz on the characterization of dielectric properties by electroreflectance and impedance measurements is particularly well done. Brief chapters on surface spectroscopy by D. K. Chakraborty, on doping level effects by M. Sharon, and by thin-film

deposition methods by S. R. Jawalekar follow. These chapters are aimed at the beginner and can be criticized only in that they lack extensive referencing of research applications of the techniques. Three contributions by Akira Fujishima on the characterization of the semiconductor interface in contact with electrolyte follow. Methods for determination of action spectra, quantum efficiencies, surface states, band-edge positions, and stability of electrodes are discussed. The style contrasts with the previous contributions in that these chapters represent detailed description of a particular system and are not so geared to the beginning student.

The chapters by Dr. Santhanam on voltammetric measurements and by Dr. Sharon on the preparation of thin films provide the theoretical underpinnings for the laboratory experiments conducted later in the book. Several applications of photoelectrochemical cells in the characterization of interfacial photoelectrochemistry (by K. Rajeshwar), photoelectrosynthesis (by K. S. V. Santhanam), the photoelectrolysis of water (by A. Q. Contractor), and a solar rechargeable battery (by M. Sharon) give brief depictions of some practical consequences of photoelectrochemistry. All four chapters are very introductory, and in their brevity they often are imprecise in introducing concepts relevant to the applications. Of particular note is the absence of a working definition for photocatalysis. The use of this term in the applications section seems quite different from that included in the preliminary overview chapter.

The laboratory experiments are a very interesting inclusion for the UNESCO Workshop. They would clearly be of benefit to the student since they represent hands-on manipulation of the equipment necessary to conduct photoelectrochemical measurements. The construction of a linear-sweep voltammetry unit, while useful from a pedagogical point of view, is perhaps not necessary for a researcher with an adequate undergraduate electrochemical background who is interested in moving into photoelectrochemistry. However, a familiarity with techniques for the fabrication of electrodes and for the measurement of band gaps, power efficiencies, and band edges is very useful. I worry, though, about the brevity of the laboratory instructions from the material given in the text. The section dealing with construction of power curves, for example, instructs the reader to measure the photopotential and photocurrent of various resistances, to plot current-potential curves, and to calculate the fill factors with no further detail. It may have been useful as well to include some sections on actinometry and the measurement of quantum efficiency in such devices.

The final chapter, by Yu. V. Pleskov, considers the realistic problems that must be faced if semiconductor photoelectrochemistry is to be considered a viable solar-energy conversion method. The problems are well laid out and are effective at introducing the beginner to important research questions.

The book is adequately, although not extensively, indexed.

Overall, the text provides a valuable and concise introduction to questions relevant to the construction of photoelectrochemical solar cells. The chapters are aimed at an audience of scientifically literate chemists or physicists who lack previous experience in this area. The text will be of less use for researchers active in the field who seek an up-to-date summary of research progress in the various topics proposed. The chapters are a bit uneven in effective documentation and in clarity. This reviewer would guess that the Workshop on which the text is based was highly successful in introducing scientists to the techniques of photoelectrochemistry and would urge that the book be considered by those seeking an initiation to the field.

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Advances in Chromatography. Volume 26. Edited by J. Calvin Giddings, Eli Grushka, and Phyllis R. Brown. Marcel Dekker, Inc.: New York. 1987. 424 pp. \$69.75. ISBN 0-8427-7664-X.

The contents of Volume 26 vary from reviews of general interest (RPLC of Sulfur and its Compounds [56], Retention Indices in Reversed-Phase HPLC [145], Retention Data for Qualitative Analysis in Capillary GC [2501]) to those for very specific applications (Fleuret Devices in GC Instrumentation [34], Hydrophobic Interaction Chromatography of Proteins [42], HPLC for Therapeutic Drug Monitoring and Determination of Toxicity [592], Element-Selective Plasma Emission Detectors for GC [82], HPLC of Neurotransmitters and their Metabolites [153]). The number in brackets after each subject refers to the number of literature citations given.

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