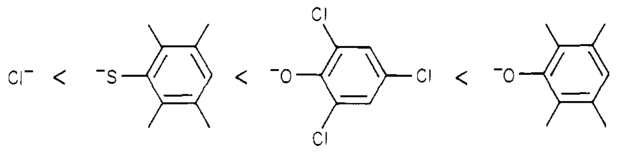

With the exception of catalase,[3] the details of the coordination geometries of the Fe(III)-tyrosine proteins have not been established. None of the known enzymes appears to contain a Fe^{III}-(tyrosine)$_4$ coordination unit. However, the coordination of multiple tyrosines to iron has been indicated in the transferrins,[4] uteroferrin,[16] and the catechol dioxygenases.[17] Further efforts to synthesize models for the Fe-tyrosine proteins are in progress.

Acknowledgment. This work was supported by grants provided by the donors of the Petroleum Research Fund, administered by the American Chemical Society.

Supplementary Material Available: Tables of fractional coordinates and thermal parameters (5 pages). Ordering information is given on any current masthead page.

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(16) Antanaitis, B. C.; Strekas, T.; Aisen, P. *J. Biol. Chem.* **1982**, *257*, 3766–3770.

(17) Que, L.; Epstein, R. M. *Biochemistry* **1981**, *20*, 2545–2549.

Book Reviews

Advances in Chemical Physics. Volumes 41 and 46. Edited by I. Progogine and S. A. Rice. John Wiley & Sons, Inc., New York. 1981. Volume 41: $60.00. Volume 46: $47.50.

Since its inception many years ago, the "Advances in Chemical Physics" series has maintained admirably high standards in its review of current research developments. Volumes 41 and 46 are welcome additions in this tradition.

Volume 41 begins with a discussion by J. S. Rowlinson of the "penetrable sphere" models for simple fluids which he and Widom first introduced over 10 years ago. Rowlinson presents a current perspective on these ideas after arguing the need for continuous—as opposed to discrete (e.g., "lattice gas")—models for the two-phase fluid equilibrium. Upon reviewing the various exact results and general approximate treatments, the article closes with specific application to the gas–liquid surface. The second contribution is by A. K. Rajagopal, who provides a comprehensive discussion of the density-functional approach to inhomogeneous electron systems, including his original work on extensions of this method to explicitly spin-dependent properties and relativistic systems. Next, F. W. Wiegel and A. J. Knox present a concise review of statistical mechanical theories of lipid monolayers. After commenting on the relevance of these systems to our understanding of the structure and function of real biological membranes, they outline recent progress on exact analyses (in two dimensions, e.g., "dimer" models), numerical simulations, and mean-field theories of the "solid", "liquid", and "gas" phases of the monolayers. The chemical reaction $F + H_2 \rightarrow HF + H$ is discussed next, by J. B. Anderson, as a test ("with more 'character' than $H + H_2 \rightarrow H_2 + H$") of our ability to calculate intermolecular potentials and collision dynamics; the relevant rate measurements and determinations of product state distribution are reviewed as stimuli for these theoretical efforts. Similarly, in an article on radiationless decay processes of small polyatomics in low-temperature solid hosts, V. E. Bondybey and L. E. Brus describe the several experimental techniques which have recently made possible the test of matrix-induced vibrational and electronic relaxation theories for guest molecular species. The theory of excitonic absorption and energy transfer in finite systems ("crystallites") is presented in the following article, by C. Aslangul and P. Kottis. This distinctly formal discussion addresses the fundamental difficulties inherent in treating interacting systems whose properties depend explicitly on the number of sites (i.e., molecules). Finally, S. L. Bernasek reviews new experimental methods for studying elementary chemical reactions which occur on well-characterized solid surfaces.

Volume 46 offers a still more theoretically oriented, and less eclectic, collection of papers. First, L. Frommhold presents a critical discussion of the extent to which ten years of collision-induced ("translational Raman") scattering measurements have allowed us to deduce information about the polarizabilities of interacting pairs of noble gas atoms. The onset of "chaotic" ("irregular", "unstable") motions in nonlinear dynamical systems is discussed next by M. Tabor. His emphasis is on the basic concepts and methods underlying the transition from regular to irregular behavior, rather than on specific applications to real molecular instances of vibrational energy redistribution. R. Kosloff then offers a necessarily abstract discussion of quantum mechanical models for "nonideal" measurements—ones which involve partial resolution and destruction. His article is followed by M. Suzuki's which outlines current theoretical ideas for treating the relaxation of arbitrary unstable states in many-body systems far from equilibrium; general scaling ideas are used to describe the roles of random forces, initial fluctuations, and nonlinearity in controlling the decay of transients. Applications to superradiance and nucleon transport, and extensions of the scaling treatment to multiplicative stochastic processes, are considered. J. S. Rowlinson's paper on the equilibrium properties of the liquid–gas interface (Volume 41) is complemented nicely by the penultimate contribution to Volume 46. Here M. S. Jhon and J. S. Dahler outline the kinetic theory of inhomogeneous fluids, discussing both formal and approximate approaches to the dynamics of the liquid–gas surface. Finally, in a break from the "physicists's systems" treated in all of the above-mentioned articles, A. Ikegami discusses statistical thermodynamic models for the denaturation ("unfolding") of proteins.

William M. Gelbart, *University of California/Los Angeles*

Analytical Chemistry of Polycyclic Aromatic Compounds. By Milton Lee (Brigham Young University), Milos V. Novotry (Indiana University), and Keith D. Bartle (University of Leeds). Academic Press, New York. 1981. xi + 462 pp. $60.00.

In this book the authors present an extensive literature review of the environmental chemistry and analytical chemistry of the polycyclic aromatic compounds (PACs). The compounds considered are the polycyclic aromatic hydrocarbons, the analogues of these in which N, O, or S replace carbon atoms in the fused-ring system, and alkyl-substituted PACs. The primary emphasis of this book is on the analytical chemistry of the PACs. Discussions are organized according to analytical methods which have been proven to be useful. Following a chapter on methods for sample collection and preliminary workup, the applications of the techniques of column, paper, thin-layer, high-performance liquid, and gas chromatographies to PAC analyses are discussed followed by chapters concerning the approaches of mass spectrometry, UV and luminescence spectroscopy, and nuclear magnetic spectroscopy. The book also contains very useful chapters concerning other aspects of the environmental chemistry of the PACs such as their occurrence, toxicology, metabolism, and physical properties.

The general quality of each of the above reviews is excellent. The authors have included an immense quantity of literature while highlighting each subject with well selected, well organized sets of examples. The result is a very readable, yet exhaustive account of the field through 1978. While the book is primarily intended for research chemists involved in PAC environmental effects and analysis, it may also be useful as a course guide for an advanced study in trace organic analysis where the PACs provide a challenging example-set of analyte molecules.

Eric Grimsrud, *Montana State University*

Acute Toxicity in Theory and Practice: With Special Reference to the Toxicology of Pesticides. By V. K. Brown (Shell Research Ltd., Kent). John Wiley and Sons, Chichester, U.K. 1980. ix + 159 pp. $28.00.

Although its title sounds rather technical and academic, this short book reads as easily as an essay or the text of a lecture. It is concerned with toxicity per se rather than toxins and is broadly directed towards students of toxicology, people in scientific administration and regulation, and people associated with pesticide R&D or use. At the outset important terms such as "toxicity", "hazard", and "acute" are defined with clarity and context. The second chapter outlines the types of toxic responses which occur, methods for their quantitative expression, and hazards of extrapolating this information. Chapters 3–5 illustrate how the outcomes of toxicity tests, which are intended to have predictive value, can be influenced by such variables as choice and status of test species, dose and mode of administration of test compound, and the hazard posed by exposure to, as opposed to administration of, real and potential toxins. Numerous brief examples are given and references to the original literature are extensive. The final chapter attempts to put the strengths, limitations, uses, and misuses of acute toxicity test results in a common sense perspective.

Robert P. Hanzlik, *University of Kansas*

Theoretical Chemistry. Volume 4. Senior reporter C. Thomson (University of St. Andrews). The Royal Society of Chemistry, London. 1981. vii + 177 pp. $86.00.

The present volume comprises three chapters: Many-body Perturbation Theory of Molecules (S. Wilson), The Electronic Structure of Polymers (J. Ladik and S. Suhai), and Electron Density Description of Atoms and Molecules (N. H. March). The exposition of these topics is uniformly well-developed, serving as an excellent reference source for theoreticians already working in the given area or as a suitable introduction for others. The section dealing with perturbation theory includes the mathematical formulation of the theory, both idagrammatically and algebraically, and computational details. Typical applications, including the calculation of electron correlation energies, are discussed as well as suggestions for future investigations. In the chapter on polymers, details are presented on the application of the Hartree–Fock LCAO approximation to crystals as well as on the use of semiempirical methods in crystal studies. Illustrative exampls are given, including the application to polyenes, infinite stacks of TCNQ and TTF molecules, and periodic DNA and proteins. The last chapter of the book deals with a technique especially appropriate to large many-electron systems and based upon the Thomas–Fermi model. The essential mathematical details are presented in a thorough fashion. Discussed in this chapter are such subjects as ionization energies and electron affinities, molecular binding, molecular vibrations, correlation energy, and topology of molecular charge distributions, among others.

M. M. Heaton, *New Mexico State University*

Metals in Biochemistry. By P. M. Harrison and R. J. Hoare. Chapman & Hall and Methuen, Inc., New York. 1980. 80 pp. $5.95.

This book is another addition to a series of short surveys entitled "Outline Studies in Biology". The books in this series are designed for the student of biological science at the late undergraduate to early graduate level. The purpose of these books is to acquaint the reader with the up-to-date results of a given area of research.

This offering deals with the broad and recently very active area of metal ions in biological systems. An introductory chapter contains a discussion of some of the properties of the essential metals of life and their role in evolution. The first major chapter is concerned with the nonredox metals (Na, K, Ca, Mg, Mn) which participate in enzyme structure and in regulation of enzymatic reactions. The following chapter deals with transition metals (Fe, Cu, Mo, Mn, Co) that are found in redox systems such as the blue copper proteins, the iron sulfur proteins, nitrogenase, and others. Oxygen binding and activation (biological conversions of O_2) by iron and copper systems are considered next. And finally, Chapter 5 contains a succinct description of the metabolism of these metals by animals.

Throughout the book, the physiological roles of the particular metal ion systems are pointed out, which allows one to obtain an overview of how metal ions participate in animal life. The large volume of material covered in this book requires that only a very brief account of individual metalloprotein systems be given. For this reason, the authors are forced to change topics rapidly, which makes it somewhat difficult to read.

This book should not be considered for use as a primary textbook for bioinorganic chemistry courses but rather as a supplementary text. The format lends itself readily to use as a study guide, possibly in preparation for cumulative examinations, since only the major results associated with a particular metal ion system are discussed.

Richard S. Himmelwright, *Polaroid Corporation*

Molecular Symmetry and Spectroscopy. By Philip R. Bunker (National Research Council, Canada). Academic Press, New York. 1979. xv + 424 pp. $33.00.

Group theory as applied to quantum mechanics has been a basic tool of molecular spectroscopists for more than half a century. Thus any new textbook devoted to this topic must offer a fresh perspective. Here is one that does. The development is based upon the complete nuclear permutation and inversion (CNPI) group, the elements of which commute with the *total* molecular Hamiltonian. This is substantially more complex than the conventional approach which focuses on the molecular point group, the elements of which only commute with the electronic Hamiltonian of the molecule in an equilibrium configuration.

From Bunker's point of view phosphine, ammonia, and BF_3 are to be initially treated as isomorphic and described in terms of a CNPI group equivalent to D_{3h}. The physical fact that inversion is essentially impossible in phosphine must then be used to transform the basis for description of its molecular energy levels to the group C_{3v}. What is the advantage of this perspective? To a student whose only interest is the electronic energy of a molecule in an equilibrium nuclear configuration (whether ground or excited state), the answer is none. To a spectroscopist who wants to interpret spectra depicting transitions between rovibronic states, the answer is a great deal. The molecular symmetry may change as a molecule is vibrationally excited (as is the case for inversion in ammonia); in terms of the CNPI group the doubling of vibronic levels in umbrella motion in ammonia appears naturally. Molecules may have different symmetry in ground and excited states, as in the $\tilde{A} \leftarrow \tilde{X}$ transitions in ethylene; again the CNPI group provides a better starting point for analyzing the transitions than does either the D_{2h} or D_{2d} group. Whenever transitions interconvert equivalent nuclear configurations, discussion based upon the CNPI group is more natural than one based upon a molecular point group appropriate to the lowest rovibrational state.

The author's approach to group theory and quantum mechanics leads from the general to the particular. It is thus too difficult for someone who has not previously studied both group theory and quantum mechanics. However, for scientists who must deal with real spectroscopic problems, not introductory simplifications, this book provides a valuable addition to the field. In addition to the development of the subject matter there are about 30 problems (with solutions) scattered throughout; these may be used by the reader to test his or her understanding of the material.

Peter C. Jordan, *Brandeis University*

Ozonation in Organic Chemistry. Volume 1. Olefinic Compounds. By Philip S. Bailey (University of Texas). Academic Press, New York. 1978. xiv + 272 pp. $30.50.

The first references in the bibliography to this volume are to Homer's "Iliad" and "Odyssey". The blind poet not surprisingly had a keen sense of smell and identified ozone during lightning storms. Professor Bailey, a long contributor to ozone chemistry, maintains this historical thoroughness and scholarly tone in the ensuing pages as well.

The topic is the reaction of ozone with alkenes. The first 100 pages are devoted to the Criegee mechanism of the reaction which evolved during the period 1949–1957. A full discussion is presented of extensions to this scheme and alternative mechanisms (some no longer extant) which were forwarded between 1966 and 1978 when the rationalization of stereochemical results was assiduously debated. Subsequent chapters describe the conversion (work up) of peroxidic products, anomalous reactions (e.g., allylic compounds), and special alkenes (e.g., allenes or hindered alkenes). The final chapter briefly reviews the reaction in the gas phase.

This treatise is not intended to be a practical manual for the working chemist nor an uncritical compilation of previous work. It is a substantive and scholarly compendium of the ozonolysis reaction (over 700 references) with emphasis on mechanistic concepts. Besides providing a perspective on past work, it should guide practical efforts to become more rational and productive. The odyssey of this reaction will be continued in a second volume which should appear in 1982. It promises to deal with acetylenic, aromatic, and heterocyclic compounds, carbon–hydrogen bonds, carbon–nitrogen double bonds, organometallics, and a variety of other topics including an update on progress with olefinic compounds.

Robert L. Kuczkowski, *University of Michigan*

Patty's Industrial Hygiene and Toxicology. Third Revised Edition. Volume 2B. Toxicology. Edited by G. D. Clayton and F. E. Clayton. Wiley-Interscience, John Wiley & Sons, New York. 1981. xx + 937 pp (2879–3816). $70.00.

This latest revision of the classic Patty's series is a "must" for those with an interest in the fields of occupational health, toxicology, or industrial hygiene.

This volume is the second of a set of three which deals with the general subject of toxicology. It comprises 11 chapters, starting with a timely examination of occupational carcinogenesis. Other chapters provide a topical focus on: the halogens and the nonmetals, boron and silicon; alkaline materials; fluorine-containing organic compounds; *N*-nitrosoamines; aliphatic and alicyclic amines; aromatic hydrocarbons; halogenated aliphatic hydrocarbons containing chlorine, bromine, and iodine; and halogenated cyclic hydrocarbons. Both an extensive subject index and a chemical index (with CAS numbers) complete this volume. While the price is a bit steep, this volume and its companions are highly recommended.

William C. Kuryla, *Union Carbide Corporation*