Additions and Corrections

Theoretical Study of the Reactions of Pentacoordinated Trigonal-Bipyramidal Compounds: PH_5, PF_5, PF_4H, PF_3H_2, PF_4CH_3, $PF_3(CH_3)_2$, $P(O_2C_2H_4)H_3$, $P(OC_3H_6)H_3$, and $PO_5H_4^-$ [*J. Am. Chem. Soc.* **1992**, *114*, 16-27]. H. WASADA* and K. HIRAO

An important report[1] on the stability of pentacoordinated phosphorane has come to our attention, which should have been cited in our reference. In this report the concept of equatophilicity, i.e. the less electronegative group prefers the equatorial position to the apical position, which is similar to our equatoriphilicity, is used to discuss the stability of trigonal bipyramids. We are grateful to Professor K. Morokuma for bringing this work to our attention.

(1) (a) Morokuma, K.; Mathieu, S.; Dorigo, A. E. *The 1989 International Chemical Congress of Pacific Basin Societies*, **1989**, phys590. (b) Mathieu, S.; Morokuma, K. *Annu. Rev. Instit. Mol. Sci.* **1990**, 18.

Book Reviews

Specialist Periodical Reports. Volume 12B. Electron Spin Resonance. Edited by M. C. R. Symons (University of Leicester). The Royal Society of Chemistry: Cambridge, England. 1991. xii + 258 pp. £105.00. ISBN 0-85186-891-6.

Specialist Periodical Reports was developed to provide research workers with comprehensive coverage in specific research areas. The *Electron Spin Resonance* (ESR) series has provided such coverage since Volume 1 in 1973, covering literature from January 1971. The field of ESR continued to grow, and in 1986, with Volume 10, the ESR series was divided into two separate books. Generally, the A series covers organic and bioorganic ESR, while the B series covers inorganic and bioinorganic ESR. However, certain topics could be placed equally well in either volume. The selection of topics has been well chosen to keep ESR spectroscopists abreast of the current literature. In addition to standard topical areas, reviews of important areas that are less proliferated with publications are included from time to time. In Volume 12B these are ESR Studies of Zeolites, ESR Imaging, and Laser Magnetic Resonance, last covered in this series in Volume 8. The usual review of theoretical aspects of ESR was postponed for 1 year. ESR literature is covered through mid-1990.

Volume 12B has 6 chapters, with five more appearing in Volume 12A. Chapter 1, Transition Metal Ions, covers spectrum analysis, phase transitions, paramagnetic ligands, mixed valence systems, three-dimensional exchanging systems (called extended systems in this chapter), semiconductors, superconductors, and the standard d^1 to d^{10} transition metal ions. The authors who have taken over this topic have done a good job in keeping the format similar to recent reviews but have also added some topics. These new subjects are provided with some background information. The older topics are not as well linked to previous reviews as in the earlier volumes, probably because of the change in authorship. This is compensated by the fact that the authors provide coverage beyond merely ESR with material and analysis that is relevant to the problem area.

Laser Magnetic Resonance (LMR), Chapter 2, was last reviewed in *Specialist Periodical Reports* when it was a fairly new technique. The last published review of this research area appeared in 1985. Therefore, this is a very timely addition to the series. This chapter provides comprehensive coverage of the results of measurements on atoms, diatomic hydrides and non-hydrides, triatomic hydrides and non-hydrides, and larger radicals. Recent theoretical work, experimental developments, and applications of the technique, principally to kinetic studies, are also covered. Current LMR work is compared to earlier work using the other kinds of spectroscopy, and background information is provided so that a non-specialist reader can appreciate the significance of the work.

Chapter 3, ESR of Transition Metal Ions in Zeolites, is new to *Specialist Periodical Reports*, but is an area that has had much attention. The literature from 1985 is covered. Short background sections covering zeolites and methods of introducing metal ions into zeolites are followed by a systematic review organized by transition metal. Some of the difficulties and ambiguities of various studies are pointed out.

Metalloproteins, covered in Chapter 4, has been a continuing topic in *Specialist Periodical Reports*. As in previous volumes, the coverage is very thorough and readable. The author includes numerous studies by non-ESR methods that are relevant to the specific metalloproteins.

Imaging by ESR methods, reviewed in Chapter 5, is a topic that is receiving progressively greater interest and is new to *Specialist Periodical Reports*. The chapter provides a good qualitative review of the area with extensive documentation, but detail that would enable a reader to select among the myriad references for particular information is not given. The topics covered include approaches to ESR imaging, instrumentation, and applications to a variety of problems of current interest, such as radiation defects, materials science, and living systems.

Inorganic and Organometallic Radicals, Chapter 6, continues from the previous volume (11B). Literature from July 1988 to August 1990 is covered. The chapter is broken into the following topics: Trapped and solvated electrons; atoms and monatomic ions; diatomic, triatomic, tetraatomic, and pentaatomic radicals; other (larger) radicals; spin trapping; and transition metal carbonyl radicals. This chapter maintains good continuity relative to earlier reports that have been published, and the figures and diagrams are well chosen to explain important issues.

In summary, Volume 12B is an important source of information on ESR. It is more than merely bibliographic information because it contains information that links work from mid-1988 (or earlier for some chapters) through mid-1990 to earlier work, gives significance to the published information, and, with its 1596 references, is an excellent directory to the primary sources. Its high cost, while commensurate with its high value, precludes many individuals form obtaining personal copies, but it is an important addition to those chemistry and physics libraries able to afford it.

Ira B. Goldberg, *Rockwell International Science Center*

Factor Analysis in Chemistry. Second Edition. By Edmund R. Malinowski (Stevens Institute of Technology, Hoboken, NJ). Wiley-Interscience: New York. 1991. xii + 350 pp. $55.00. ISBN 0-471-53009-3.

Every head or a chair of a chemistry department should read the first (Introduction) and the last (Additional applications) chapters of this book and then try to answer the following question: Do we have an expert in this field of chemistry, or at least, anyone in my department who is

sufficiently familiar with this subject? The rest of chemical community should read the chapters in-between, according to their professional interest. It is an apparent absurdity of our times that so much money and efforts are invested in acquiring instrumentation of ever increasing precision and power and at the same time so little money and manpower are invested in efforts to intelligently digest the accumulated information. Factor analysis is one of the prime methodologies for data reduction, and this book outlines the underlying mathematics and computational details involved while illustrating these with numerous examples from chemistry. The book will be particularly welcome as it gives enough background to users of various available statistical packages, such as SAS and SPSS (Statistical analysis system and Statistical Package for the Social Sciences, respectively), which may demystify in part their use as "black boxes".

This edition of *Factor Analysis in Chemistry* is an update of the first edition, which appeared 10 years ago. Most of the changes concern chapters on advanced computational aspects (Effects of experimental error, Numerical examples, and Special methods). The introductory parts (Introduction, Main steps, and Mathematical formulation) as well as the chemical applications (Component analysis, Nuclear Magnetic Resonance, Chromatography, and other applications) remain essentially unchanged.

After this initial praise of the book for the chemical community at large (the book is well-written), let us point to some critical comments, which speak more of what is not in the book than what is. The statement found in the opening section, "Factor analysis (FA) was founded by the behavioral scientists", is at best an exaggeration. FA was founded by a behavioral scientist (singular), as clarified in a subsequent sentence "The first real development was accomplished by Hotelling, in 1933." I mention this for two reasons: first, to impress on chemists how late we are in enriching our own chemical analyses with available methodologies, which only since 1970 have been recognized by chemists as important, and second, while perhaps the words "the Principal Component Analysis" (PCA), which in many aspects overlap with Factor Analysis, are household words in certain chemical circles, few have heard of Hotelling. Yet, just as Dunzig is the sole pioneer of Linear Programming, and Shanon of the Information Theory, one may say that Hotelling is the founder of Factor Analysis.

The book could have benefited from mention of several classical applications, particularly from the area of structure–property and structure–activity studies. Among two-dozen acronyms scattered over the book one does not find QSAR (quantitative structure–activity relationship). Although a large part of QSAR uses multivariate regression, a sizable part of the literature (e.g., Jurs, Cramer, Miyashita, Basak) is concerned with the applications of factor analysis. Medicinal Chemistry deserves more than 2 pages of the book. Even more striking is the lack of any reference to graph theoretical (topological) and other structural descriptors (which are mathematical invariants of a molecular graph or a molecular structure) in such studies. They are of interest if one wants to give more attention to the *interpretation* of the results, i.e., interpretation of individual principal components (vectors). In the last 10 years we have seen impressive developments in this very area, but perhaps they have to wait for the third edition. Of course, a book of 350 pages (and at a very reasonable price) cannot perhaps adequately discuss the "omitted" material. However, it is somewhat disappointing that so little space was devoted to interpretation of the principal components—since here PCA is deficient, and users should be alerted to that. Even a browser through the literature on factor analysis may have observed the paradoxical situation that fine quantitative results (principal components) are only explained in very qualitative terms (such as "bulk", "cohesiveness"). Recent developments on the resolution of ambiguities in structure–property studies by use of orthogonal descriptors (*J. Chem. Inf. Comput. Sci.* **1991**, *31*, 11), which have been published since the book was in print, may help readers to overcome some of these difficulties in the interpretation of principal components.

Milan Randić, *Drake University*

Chemical Analysis. Volume 117. Applications of Fluorescence in Immunoassay. By Ilkka A. Hemmilä (University of Turku, Finland). Edited by J. D. Winefordner. Wiley: New York. 1991. xi + 343 pp. $85.00. ISBN 0-471-51091-2.

Fluorescence in immunoassay methodology might be called the technique of the future and, facetiously, always will be. This text is a thorough survey by an important practioner in the field of how present the future has become. Dr. Hemmilä has previously written important reviews of this area, and this text builds on those and broadens their scope considerably. To call this survey thorough is a considerable understatement encompassing as it does 1919 references (most cited as individual items) on virtually all aspects of the components of this field. This breadth and detail found in 248 text pages obviously preclude lengthy exposition on very many individual topics. The author's goal and reader's results are a thorough acquaintance with virtually everything of significance in the field. In depth pursuit of topics is at the readers initiative, and ease of access is excellent through the referenced work.

The nature of the coverage in all topics includes theory and historical progression of the subfield's development up to the state-of-the-art, with continuous reference to fluorescence immunoassay. Both research level results and techniques are included, along with comparisons of alternative technologies. Topics include, besides fluorescence immunoassays, chapters on antibodies, immunoassays, photoluminescence spectroscopy, instrumentation available, fluorescent probes, fluorometric enzyme immunoassays, non-immunological specific binding assays, and multiparametric assay design.

Chapter 2 (after a 2-page introduction) is a short (20 pages) primer on antibodies including immunogenicity, polyclonal vs. monoclonal antibodies, structure, and isolation. Also included are immunoassay conditions dictated by these antibody characteristics and an introduction of other specific binding proteins. Though very basic, the material is constantly related to immunoassay.

Chapters 3 and 4 (28 pages) concern the basics of immunoassays and their historical development up through the rising dominance of nonisotopic labels. Chapter 5 (26 pages) is about the basics of photoluminescence theory, including the factors affecting sensitivity limits of fluorophore detection. Instrumentation is covered in Chapter 6 and includes both theory and mention of all commercially available instruments.

A surprisingly extensive (60 pages) review of the various classes of photoluminescent probes including organics and organometallics is found in Chapter 7. This discussion includes properties, spectra, conjugation to immunological components, and application to fluorescence immunoassay. Chapter 8 constitutes the heart of the text (55 pages) and includes all approaches to heterogeneous, non-separation, and time-resolved fluorescence immunoassay. Research level approaches are included along with those with commercial embodiments. The text concludes with three short chapters on enzyme immunoassays with detection by fluorescent product formation, other specific binding assays including DNA hybridization detection, and a very short look at the suitability of fluorescence as the probe for single assays designed to detect multiple analytes.

In summary, this text serves well a mixed audience from neophyte to those with considerable expertise in need of a thorough literature review. It blends nicely a research and commercial focus.

Keith J. Schray, *Lehigh University*

Continuous Flow Methods in Organic Synthesis. By P. Tundo (University of Venice). Ellis Horwood: Chichester, U.K. 1991. 378 pp. $130.00. ISBN 0-13-170788-4.

This is a clearly-written and well-illustrated single-author review text, with a title which at first sight suggests that it might be directed, in the main, at chemical engineers. In fact, this is an oversimplification, and indeed a large amount of what the book has to convey is directed toward synthetic chemists. From this point of view, the book is rather unique and describes those developments lying somewhere between chemical and process engineering and synthetic organic chemistry, where continuous flow methods have brought some real advantage to the synthesis. Perhaps implicit in the book as well is the message that there is great scope for synthetic chemists to consider the downstream consequences of their chemistry while actually in the act of developing new chemical methodology. This might not only lead to more efficient technological exploitation of new chemistry, but it may also point out the folly of certain lines of research in terms, for example, of their inevitable longer term environmental consequences.

Following a brief introduction in which the author familiarizes the reader with some well-known heterogeneous processes, Chapter 1 describes the preparation and properties of heterogeneous and heterogenized catalysts. Reactions are categorized as gas–solid, gas–liquid and liquid–solid, and the various solid supports used are described under these headings. The synthesis, structure and application of metal oxides, zeolites, kieselguhr, celite, porous glass, carbons, and organic polymers are covered in this way, where the emphasis is on the solid component rather than the reaction. In the course of this, however, reactions as diverse as oil cracking and peptide synthesis are included. This is undoubtedly a key chapter, and in terms of describing the heterogeneous or heterogenized species lays the foundation for the chapters which follow. This is reflected in the number of literature citations, 384, some dated as recently as 1991.

Chapter 2 deals with the characterization of supported catalysts. This is a very difficult area and one often avoided by researchers as a result. Surface chemists might be disappointed with these pages because they are not bogged down with modern surface analytical data, but focus on the more practical parameters which are of concern to catalyst users.

Chapter 3 goes into more detail about the *reactions* carried out in the gas phase over solid catalysts. It deals not only with technologically important processes, but also other reactions and catalysts that have been researched, but not so far exploited. Similarly, Chapter 4 covers reactions carried out in the gas phase over a *liquid film* of catalyst on a solid support. Supported phosphoric acid is an important industrial example, as are vanadia melts. However, the bulk of this chapter describes the various gas–liquid phase transfer catalyzed reactions pioneered by the author and certainly developed to at least pilot-plant scale. Again, this is an important section of the book and is a unique review of this area.

Chapter 5 describes continuous-flow syntheses in the liquid phase and again has great value because of its novel and unifying treatment of a number of apparently diverse systems—solid phase peptide synthesis, sulfonic acid resin catalyzed reactions, supported phase transfer catalysts, immobilized enzymes, and asymmetric reactions. Essentially all of these topics have been reviewed more than once before, but here the emphasis is on the continuous flow methodology—what the methodologies are and what bonuses they bring to each individual chemistry.

The book is completed by three appendices—membranes and membrane reactors, monoliths, and reactors. Why these had to be designated as appendices is unclear, because in each case they make a valuable contribution and add to the uniqueness of the text. Possibly the author did not want to convey any misconception that these were weighty, state-of-art descriptions, rather than descriptive overviews to complement his main text.

Overall, Professor Tundo has to be congratulated; he has produced a stimulating and unique text, *a reading of which would benefit all synthetic chemists*. No doubt the more broadly thinking chemist in industry will be attracted by the title and be prepared to invest some time, at least in scanning the work. Synthetic chemists in academia are less likely to be impressed, and they will be the losers for it.

D. C. Sherrington, *University of Strathclyde*

Gel Electrophoresis of Proteins: A Practical Approach. Second Edition. By B. D. Hames (University of Leeds) and D. Rickwood (University of Essex). IRL Press: Oxford. 1990. xviii + 383 pp. Hardback: $75.00. ISBN 0-19-963074-7. Paperback: $50.00. ISBN 0-19-963075-5.

This book represents an extremely well-written, easily followed, comprehensive treatise of the practical aspects of protein electrophoresis. The book is divided into five chapters, each written by a highly regarded expert in their respective fields, and an appendix section. The first chapter by Hames presents a concise yet thorough treatment of one-dimensional polyacrylamide gel electrophoresis. This chapter is the longest in the book covering most of the recently developed methods for the analysis of gels, including the uses of different radiolabeling, staining, and blotting techniques. Subsequent chapters present detailed descriptions of the other major electrophoretic procedures including both conventional and the most recently developed immobilized pH gradient isoelectric focusing applications (Righetti), two-dimensional polyacrylamide gel electrophoresis (Rickwood), with a brief introduction to computer assisted analysis of 2D electrophoretograms, immunoelectrophoresis (Bøg-Hansen), and peptide mapping (Andrews). The final section, the appendix, provides a wealth of information concerning supplier sources, polypeptide detection methods, reagents for isotopic labeling, electrophoretic standards, and applications of two-dimensional gel electrophoresis and immunoelectrophoretic techniques. This book represents an indispensible reference source of both background and practical information for anyone, both novices and experienced researchers, involved in any aspect of protein separation.

Peter J. Wirth, *National Cancer Institute*

Hydrogen Bonding in Biological Structures. By G. A. Jeffrey and W. Saenger (The University of Pittsburgh and Freie Universitat Berlin). Springer-Verlag Publishers: New York. 1991. 569 pp. $79.00. ISBN 0-387-50839-2.

The goal of this book is to present hydrogen-bonding patterns as revealed by crystal structures to chemists and biochemists. Attention is given mostly to those aspects of hydrogen bonding that yield the three-dimensional structures of biological macromolecules. A great deal of data from the Protein Crystal Structure Data Base is nicely compiled into an orderly and readable presentation. The book has already become an important reference in our group library, allowing quick and easy access to examples of several hydrogen-bonding groups. The book is broken down into several parts of increasing complexity. The first details the importance of hydrogen bonds and defines these and the experimental and theoretical methods for studying them. The next part delineates hydrogen-bonding geometries and patterns found in small often nonbiological molecules and the typical geometries of multicentered hydrogen bonds. The third part of the book extensively covers hydrogen bonds within and between small biological molecules such as saccharides, purines and pyrimidines, and amino acids. The next part builds upon this knowledge and thoroughly covers hydrogen bonding patterns in biological macromolecules built from the previously discussed monomers. Finally, the last part examines hydrogen bonding by water and the role it plays in solvating and changing the structures of the macromolecules.

The book contains nearly 450 Protein Crystal Structure Data Base reference codes and 900 references. For a book on such a vast subject, this text does a remarkably good job at organizing and presenting the material. Besides making an excellent reference book, it would also make a good text for a special topics course.

Eric Anslyn, *University of Texas at Austin*

Phase Diagrams of the Elements. By David A. Young (Lawrence Livermore National Lab). University of California Press: Berkeley, California. 1991. 291 pp. $39.95. ISBN 0-520-07483-1.

The study of phase behavior of the elements, since it involves the use of pressure as a variable, and the study of theory as it relates to the structure of solids, since it involves the consideration of translational symmetry, are not areas with which the majority of chemists are familiar. Yet the results of such experiments and of such calculations, especially as the experiment and theory are inter-related, provide a basis for a deep understanding of the elements and their periodic properties and, in a sense, a baseline for the consideration of their chemical interactions. Therefore, chemists will find this book thought provoking and useful for teaching the periodic properties of the elements. In this work, the author has brought together the experimental and theoretical information that has been obtained by experimental methods (diamond anvil, shock wave, isobaric heating) extending measurements of pressure into the hundreds of GPa and temperatures to 8000 K, and by the modern theoretical techniques of band structure and quantum-molecular-dynamics calculation. The result is a striking interplay of experiment and theory that is capably described by the author and yields an evocative collection of descriptions of structure and heterogeneous behavior.

Hugo F. Franzen, *Iowa State University*

Perspectives on Bioinorganic Chemistry. Volume 1. Edited by Robert W. Hay, Jon R. Dilworth, and Kevin B. Nolan (University of St. Andrews, UK; University of Essex, UK; and Royal College of Surgeons, Ireland, respectively). JAI Press: Greenwich, CT. 1991. xi + 284 pp. $78.50. ISBN 1-55938-184-1.

The inaugural volume of *Perspectives on Bioinorganic Chemistry* offers seven reviews. The first, by L. D. Petit, J. E. Gregor, and H. Kozlowski, deals with peptide complexes and is disappointingly incomplete. Interested readers will find relevant chapters in the *Specialist Periodical Report on Amino Acids and Peptides* series to be of greater value. T. H. Fife's review of metal-ion catalyzed ester and amide hydrolysis offers a timely and very useful discussion of issues that are of relevance to the catalytic mechanisms of hydrolytic metalloenzymes. The contribution by S. K. Chapman focuses on new developments in the bioinorganic chemistry of blue copper proteins. This review offers very little fresh insight into important issues that are outstanding; in particular, the recent review by E. T. Adman (*Adv. Prot. Chem.* **1991**, *42*, 145) contains a much more valuable discussion of structural work on these proteins. F. A. Armstrong's review of voltammetry of metalloproteins will be of interest to newcomers to this field. However, this review is largely an abbreviated version of an earlier review (by the same author) that appeared in Vol. 72 of *Structure and Bonding*. W. E. Smith and J. Reglinski present an account of developments in the chemistry and pharmacology of gold drugs used in the treatment of rheumatoid arthritis. The penultimate review, by R. C. Hider and A. D. Hall, is a well-written survey of medicinal applications of iron chelating agents. The closing contribution (by R. R. Eady) surveys the biochemistry of molybdenum-independent nitrogenases; this topic is also the subject of a review, by the same author, that appeared in Vol. 36 of *Advances in Inorganic Chemistry*. In summary, this volume contains reviews of variable quality that mostly survey the literature to 1989. There is no general index.

Two established series, *Advances in Inorganic Biochemistry* and *Metal Ions in Biological Systems*, consistently offer high-quality reviews that survey the bioinorganic field. In addition, relevant reviews routinely appear in nearly a dozen other serial publications. In view of the fiscal constraints that many research libraries face, it is difficult for this reviewer to enthusiastically recommend the acquisiton of a new serial publication such as this.

Walther R. Ellis, Jr., *University of Utah*