Book Reviews

Advanced Molecular Dynamics and Chemical Kinetics. By Gert D. Billing and Kurt V. Mikkelson (University of Copenhagen). John Wiley: New York. 1997. xiii + 288 pp. $54.95. ISBN 0-471-12740-X.

The back cover of this book announces that "This is the first book of its kind to combine all the theories of molecular reaction dynamics and chemical kinetics in a single source". The authors, who are active and accomplished researchers in the field, are more honest in their preface, where they write "Our intention has been to present a selection of methods...". They go on to write that "...the book contains a great many subjects-perhaps too many..." and further "Some topics are presented, if only briefly, because we consider it to be important to have at the very least a superficial knowledge of some of these techniques...".

This slim volume of 20 chapters, including an introductory chapter, emerged from graduate courses taught by the authors. It is a two-part book, with the first part written presumably by Billing and the second part written by Mikkelson. The longest chapter is the second one, where 30 pages are devoted to the elements of second quantization—not, in my opinion, among the more important theoretical tools used in the theory of chemical dynamics and kinetics. The remaining 19 chapters average 11.6 pages, but with 4 or 5 chapters only 7 or 8 pages in length. Chapters 3−12, the Billing chapters, range from broad topics such as semiclassical theories (16 pages), potential energy surfaces (7 pages), quantum theory of rate constants (10 pages), to more specialized ones on photodissociation (14 pages), and the reaction path method (8 pages). Billing writes in many places with insight and real clarity. Also, a short set of solved problems in these chapters (with the strange exception of Chapter 12 which does not have solutions to the problems) is a real plus. Chapter 13, Evolution of a total system (5 pages), is, I gather, the bridge to the remainder of the book, Chapters 14−20, written presumably by Mikkelson. These chapters deal with events in solution, with a focus on electron transfer. They are quite different in style, and owe very little to the preceding chapters, with the exception of Chapter 2 on second quantization. There are no exercises in these later chapters, and the blizzard of equations often obscures physical insights and pedagogy.

Obviously I am not very enthusiastic about this book. Molecular dynamics and chemical kinetics are huge and important fields, and it is unlikely that a comprehensive book will (or could) be written on both. There are, however, some recent books that together do a reasonable job of it. These include a recent one by Baer and Hase entitled *Unimoleculear Reaction Dyanmics*, and an edited volume, *Dynamics of Molecules and Chemical Reactions* by Wyatt and Zhang. Astonishingly, neither of these books is referred to in the Billing−Mikkelson book. These and other omissions indicate that the authors were not attempting to be comprehensive in referring to the literature—and in that they succeeded. This lack, plus the mostly superficial treatment of topics, makes it difficult to recommend this book to graduate students. It might find its place in a graduate course, however, with much left for the instructor to fill in.

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Anti-infectives: Recent Advances in Chemistry and Structure−Activity Relationships. Edited by P. H. Bentley (Smith & Nephew Group Research Centre) and P. J. O'Hanlon (SmithKline Beecham Pharmaceuticals). American Chemical Society: Washington, DC. 1997. xi + 338 pp. $174.00. ISBN 0-85404-7077.

This book is a compendium of the material presented at a symposium on anti-infectives, Recent Advances in the Chemistry of Anti-infective Agents, held in July of 1996. The 23 chapters are divided into 3 categories antibacterials/antibiotics, antifungals, and antivirals, with 9, 5, and 9 contributions, respectively. In general, the coverage is complete and a good representation of the status in the field of anti-infectives. A balanced mixture of contributions from academic and industrial laboratories, with their different research goals and resources, provides for a good perspective. Detracting from the book is the typeset and font used in some of the contributions; these chapters are extremely uncomfortable to read, with text that is splotchy and extremely crowded.

In the section on antibiotics and antibacterials, the majority of the contributions concentrate on design/synthesis of the molecules. The two exceptions describe structure−activity relationships: D. H. Williams recaps his work on glycopeptides, and G. Burton describes advances on the inhibition of signal peptidase enzymes. The chapters based on design and synthesis are thorough, supplying sufficient detail, with many references to the original literature, and some hindsight into the rationale for the synthetic route chosen. Many of the old players in the field of antibiotics, including oxazolidinones and β-lactams, have been structurally modified, often using some novel chemistry, in an attempt to overcome bacterial resistance.

The second section contains contributions describing the design and synthesis of second-generation azole-based antifungal agents by groups at Pfizer, Zeneca Agrochemicals, and Schering-Plough. The description of the development of these compounds, including both the successes and failures along the way, provides insight into the many different aspects in the design of orally active, therapeutic agents against fungal infections. Other contributions include the development of benzimidazole agents targeted at tublins and novel molecules targeted against the cell-wall components chitin and glucan fibrils.

The final section covering antivirals begins, quite naturally, with an HIV protease inhibitor: in this case the development of crixivan (L-735,534, indinavir sulfate) by Merck. The contribution describes the concept and provides detailed synthetic methods. A thorough characterization of 4′-thio-2′-deoxyribonucleosides and their use as antiviral agents is provided by R. T. Walker. The incorporation of the sulfur stabilizes the N-glycosidic bond to phosphorolysis while introducing very little structural change to the nucleotide. P. Herdewijn reviews the use of nucleosides containing six-membered carbohydrates. Advances in the development of pro-drugs, to enhance the intracellular delivery, by modification of the phosphate group of AZT is detailed by C. McGuigan. The family of Tsao-T-based inhibitors of reverse transcriptase (RT) are provided by M.-J. Camarasa. The use of non-nucleotide RT inhibitors is reviewed by E. Arnold. In the contribution from P. W. Smith, novel inhibitors of influenza A sialidase based on the classic 2,3-didehydro-*N*-acetylneuraminic acid analogues are described. Along the synthetic pathway, the replacement of a carboxylic acid with a carboamide leads to a new target compound. J. S. Mills describes the development of proteinase inhibitors for viruses other than HIV-1. Utilizing the body of knowledge gained from the investigation of HIV should greatly help in the inhibition of other viral proteinases. A good example is provided by J. C. Vederas, with details of the design and synthesis of viral cysteine proteinases.

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Single-Molecule Optical Detection, Imaging and Spectroscopy. Edited by T. Basche, W. E. Moerner, M. Orrit, and U. P. Wild. Wiley/VCH: New York. 1997. $198.00. xiv + 250 pp. ISBN 3-527-29316-7.

Recent advances in ultrasensitive instrumentation have allowed the detection, identification, and dynamic studies of single molecules in the condensed phase. This measurement capability provides a new set of tools for scientists to address important current problems and to explore new frontiers in many disciplines such as chemistry, molecular biology, solid-state physics, and materials research. Now, Basche, Moerner, Orrit, and Wild have put together a book on this topic. With contributions from leading authors in the field, this book provides an excellent overview (with references) on the principles, techniques, and potential applications of single-molecule detection. It is a must-read

for anyone who is interested in applying single-molecule techniques to their own research.

The book is divided into three sections according to the techniques that are used for single-molecule detection. These techniques differ in sampling conditions and the means of delivering excitation energy, but all of them share the need to isolate single molecules for detection. One approach is to isolate individual molecules spectroscopically in low-temperature solids because matrix perturbations cause each molecule to have a slightly different absorption frequency. A more broadly useful approach is to isolate molecules on a surface or in dilute solution; that is, individual molecules are spatially separated from each other in the area or volume probed by a laser beam.

The first section deals with single impurity molecules embedded in low-temperature solids. Moerner describes the fundamental principles and experimental methods in high-resolution single-molecule spectroscopy, and Basche and co-workers discuss single-molecule excitation profiles, wavelength-resolved spectroscopy, and quantum optical studies. Wild and co-workers present fluorescence microscopy, polarization, and lifetime measurements. A fascinating finding is that the absorption line of a single molecule often undergoes frequency jumps called "spectral walking". This behavior is discussed experimentally by Brown and Orrit and analyzed theoretically by Skinner. This section concludes with the use of magnetic resonance to detect single molecular spins.

The second section covers the use of near-field scanning optical microscopy (NSOM) for single-molecule studies at room temperature. Trautman and Ambrose first discuss the fundamental principles of NSOM and then describe its applications to single-molecule imaging and spectroscopy. The main advantages of near-field microscopy are its improved spatial resolution and the ability to correlate spectroscopic information with topographic data. If the primary goal is to study single molecules and subdiffraction spatial resolution is not essential, far-field confocal and evanescent-wave methods may be better choices. Far-field optical excitation in the confocal or evanescent-wave mode is much simpler and noninvasive, and has unlimited laser throughputs.

The third section discusses single-molecule detection in the liquid phase. A number of schemes are described including hydrodynamic sheath flow, microdroplets, confocal microscopy, total internal reflection, and electrophoresis capillaries. A single molecule in solution is generally detected as a photon burst as the molecule moves across a tightly focused laser beam by either liquid flow or diffusion. These studies present an opportunity for sensitive chemical analysis without standards and are important to ultrasmall and ultrasensitive chemical instrumentation.

With the caveat that the most exciting and important insights are likely to be unforeseen, single-molecule detection and spectroscopy has already yielded new information that is not available from population-averaged measurements. In particular, discrete spectral jumps or intermittent photon emission has been observed for single dye molecules, single fluorescent protein molecules, and single conjugated polymer molecules. Still, the future of single-molecule detection appears to lie in its application to solve important problems such as DNA sequencing, biomolecular dynamics, ultrasensitive diagnostics, and optical information storage.

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Organic Reactions in Aqueous Media. By Chao-Jun Li (Tulane University) and Tak-Hang Chan (McGill University). John Wiley and Sons: New York. 1997. xi + 199 pp. $59.95. ISBN 0-471-16395-3.

The monograph *Organic Reactions in Aqueous Media* by Chao-Jun Li and Tak-Hang Chan is a wonderful resource for a broad audience. This text should be useful to not only those currently practicing the art of organic synthesis in aqueous media but all organic and organometallic chemists interested in learning about the possibilities of reactions in this unusual (for the organic chemist) environment. There are a number of features which make this a very attractive and useful volume. First, the coverage is extensive. The topics covered include pericyclic reactions, nucleophilic additions and substitutions, metal-mediated reactions, transition metal catalyzed reactions, and oxidations and reductions. There is also a separate section giving an overview of current industrial applications of aqueous organic chemistry. Hydrolysis reactions are not covered, but the authors adequately explain this exclusion in the preface. Second, each reaction is fully illustrated with very clear structural drawings. Where different stereochemistries or regiochemistries are possible in the products, full details of product distribution are typically provided. Finally, the references are fairly up to date for a book published in 1997; references from 1995 and 1996 are common. While the references may not be exhaustive, the text provides a good coverage of each topic. The only drawback to the text is that there are a number of places throughout where the grammar seems awkward and stilted. This is not a serious problem since these occasions are quite rare and do not really mar the overall effectiveness of the text. Overall, with a reasonable price for a scientific monograph, this volume is a must for researchers working in aqeuous media and highly recommended for all who are involved with organic synthesis in its broadest sense.

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Environmental Toxicology and Chemistry. By Donald G. Crosby (University of California, Davis). Oxford University Press: Oxford and New York. 1998. 336 pp. $59.95. ISBN 0-19-511713-1.

A knowledge of the chemistry of toxicants, including the biochemical and chemical transformations, is invaluable for a better understanding of their toxic effects. Hence, it is unfortunate that most books should treat environmental toxicology and environmental chemistry as two different subjects. This is probably because of the extensive nature of each subject and the requisite background in several specialized areas. It is in this context that Dr. Crosby's ambitious attempt at bringing together both these subjects in one book has to be appreciated.

The result is a work of 16 chapters which cover a wide range of topics. After introduction of the preliminaries in the first chapter, environmental chemicals and their chemodynamics, transport, and abiotic transformations are discussed in the next four. This is followed by a discussion, in Chapters 6−10, of toxicological subjects including Biotransformations, Intoxication, Quantitative Toxicology, Intoxication Mechanisms, and Exposure and Risk. In the next five chapters (11−15) examples of specific environmental chemicals (Inorganic Toxicants, Biotoxins, Industrial Chemicals, Refractory Pollutants, and Reactive Pollutants) and their toxicological effects are presented while Chapter 16 is devoted to prediction of the environmental fate and effects of toxicants. Representative examples of toxicants (both organic and inorganic in nature), their effects, their occurrence and distribution in nature or production on an industrial scale, regulatory controls by specified agencies, and a great deal of other useful information have been given in a large number of tables in the relevant sections. Literature is cited from as far back as the 1950s and as recently as 1997. At the end of each chapter an illuminating discussion of a special topic is included.

The greatest merit of this work is its readability, which is a result of the lucid, unpretentious style of writing. This feature is especially important if the book is to be used for an introductory course at the undergraduate level.

Although a simplified style is generally laudable, it can sometimes lead to inaccuracies. This drawback is evident in this book in several places, especially in discussions of some aspects of chemistry. For example, the following statements appear in Chapter 16: "Every physical or chemical system contains energy, generally expressed as heat (H)." "Free energy makes things happen." "The equilibrium and rate constants for any reaction are directly and linearly related to ...$\Delta G°$." Energy is not stored in a system as heat. Heat becomes equal to enthalpy transferred at constant pressure. Besides H is the symbol for enthalpy, not for heat. Free energy merely indicates the *possibility* that some process can take place but a kinetic barrier can preclude its happening. The equilibrium constant is related to $\Delta G°$ between products and reactants. According to the transition state theory, the rate constant is related to the Gibbs free energy change between the activated complex and reactants, but this is not $\Delta G°$. In eq 5.27 (p 81), which relates log K to $\Delta E°$, the factor 2.303 should be in the denominator, not the numerator. Water is referred to as "hydrogen

oxide" (p 84); its correct term is "dihydrogen oxide". As with most other books on cognate subjects, Detection and Measurement (Chapter 2) have been discussed superficially with a cursory mention of TLC, GLC, LC, and immunoassays and two brief paragraphs on analyte detection. Since some toxicants are routinely analyzed by GC−MS, it is surprising that mass spectrometry should be completely omitted in a list of chromatographic detectors (Table 2.2) that is titled Some Modern Analytical Detectors. Moreover, not a single technique for analysis of inorganic toxicants (e.g., atomic absorption spectrometry) is even mentioned. The difficulty of accurately measuring low concentrations has been highlighted, but the possible improvements have not even been mentioned.

In contrast, topics on toxicology constitute the stronger aspect of the book although molecular mechanisms of toxicity could have been dealt with in greater detail to avoid any confusion. For example, although binding to sulfhydryl groups may be a dominant mechanism, the toxicity of arsenic is species-dependent and may involve other mechanisms as well.

Overall, the clarity of exposition and the range of topics covered would commend this book to undergraduates as an appropriate text for an introductory course on environmental toxicology and/or environmental chemistry. Corrections to the indicated misstatements would undoubtedly enhance the utility of the next edition.

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Principles of Molecular Biology, Volume 5: Molecular and Cellular Genetics. Edited by E. Edward Bittar and Neville Bittar (University of Wisconsin). JAI Press: Greenwich, CT. 1996. xiv + 412 pp. $128.50. ISBN 1-55938-809-9.

The authors of this book have attempted to fill in an important piece of a puzzle which, regrettably, keeps changing at breath-taking speed. Because the knowledge in the field of molecular genetics is literally exploding, the authors had a difficult task of critically discussing important subjects which are in rapid flux. The volume fulfills an essential need. Specifically, it presents in a review-like format the 1995-96 state-of-the-art of the subject based on information available *at that time*. Most of the chapters are written concisely and informatively.

The topics of nucleosome structure and DNA replication are handled with clarity and enthusiasm. The chapter on DNA methylation, an important subject for most aspects of nucleic acid function, is poorly written and organized in an uninteresting fashion. The chapters on histone acetylation, synthesis and activity of transcription factors, and alternative DNA splicing are well written and presented with skill. The protein−DNA interaction subject is presented in a somewhat heavy-handed manner with exuberant description of spacial modalities but with little consideration of relevant consequences.

The potential use of antisense nucleic acid fragments for inhibition of gene expression is skillfully explored. The essential aspects of specificity, efficiency, delivery, and toxicity are well addressed. The use of antisense reagents in clinical medicine shows interesting promise in the fight against viruses and cancer.

The possible mechanism and pathways for signal transduction from external cell-membrane receptors to intranuclear DNA are presented with insight. The emphasis is mainly on the dynamic aspects of the process such as distribution and equilibria of architectural proteins and protein kinase activities. Other important aspects of transduction such as changes in cell morphology and availability of cytoloplasm-produced metabolites are acknowledged but not considered. The subject of DNA damage and repair is succinctly exposed and linked to some known hereditary human disorders in which a repair function does not conform to the normal cellular response to DNA damage.

The chapters on PCR, molecular cloning, and use of DNA probes deal mostly with standard techniques in experimental molecular genetics.

Overall, I enjoyed reading Volume 5. It covers quite satisfactorily most of the important subjects in the field of molecular and cellular genetics. Graduate students in biochemistry, molecular biology, and genetics may find the book edited by the Bittars useful and informative. The introductions of each chapter review concisely some important basic principles in the field. Unfortunately, by 1998, Volume 5 of *Principles of Medical Biology* is out of date. While this may limit its value for researchers, the book can be quite useful for trainees, graduate students, and educators.

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Plasma Source Mass Spectrometry: Developments and Applications. Edited by Grenville Holland (University of Durham) and Scott D. Tanner (PE-Sciex). American Chemical Society: Washington, DC. 1997. x + 329 pp. $136.00. ISBN 0-85404-727-1.

This book represents the proceedings of the 5th International Conference on Plasma Souce Mass Spectrometry, which was held in September 1996 at the University of Durham, U.K. There are 31 papers on ICP mass spectrometry and 1 on glow discharge emission spectrometry. The ICP-MS papers span a wide range of interests, with fundamental papers on (a) the effects of droplets and particles on the ICP, (b) space charge effects on ion optics, (c) the use of a hexapole collision cell for removing polyatomic ions, (d) a magnetic sector MS that is capable of higher spectral resolution and sensitivity than the usual quadrupole analyzer, and (e) the use of solvent removal and multicomponent analysis to deal with spectral interferences.

Applications of ICP-MS is the main theme of this conference, and some of the topics emphasized include flow injection for matrix removal and preconcentration, speciation, the analysis of biological materials such as urine, plants, and food, trace element measurements in steel, landfills, drinking water, and Antarctic waters, radionuclides in concrete, etc.

All the papers are quite current. Some are of very high impact, such as the initial description of the desolvated microconcentric nebulizer. Except for a few overview papers, each article is an original work, not a rehash of material published elsewhere. The application papers span most of the scientific uses of ICP-MS and provide a good picture of the types of problems addressed by this technique. The papers are edited to a fairly uniform format. There are very few errors, the most serious one being the statement on p 52 that a shielded plasma cannot be operated under normal "hot" conditions. A good index is provided.

This book is very valuable for the ICP-MS practitioner who wants a survey of the main new developments under a single cover. It belongs in the library of every research group or institution that is active in ICP-MS. It is not a textbook but would serve as a valuable resource for any course in analytical atomic spectrometry, in a mass spectrometry course that includes inorganic analysis, or in an instrumental analysis course. I commend the editors for a job very well done.

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Catalytic Reductive Carbonylation of Organic Nitro Compounds. By Sergio Cenini and Fabio Ragaini (Università degli Studi di Milano). Kluwer Academic: Dordrecht. 1997. xii + 340 pp. $169.00. ISBN 0-7923-4307-7.

This monograph is the 20th volume in the series Catalysis by Metal Complexes edited by Renato Ugo and Brian R. James. These generally involve comprehensive reviews of a narrowly defined topic within the field of catalysis. Such is the case with the current book. Catalytic carbonylations of nitro groups, especially for the production of isocyanates and carbamates, are of special interest as a replacement for existing phosgene-based technology. The great interest in this area originated in industrial laboratories, and a large portion of the literature is located in patents. To their credit, the authors have included a review of the patent literature, and this summary alone greatly enhances the value of this volume. Many of the catalytic systems are homogeneous and are based on soluble complexes of palladium and ruthenium. Throughout the book, the authors nicely complement the survey of

catalytic conditions, yields, etc. with potentially relevant stoichiometric chemistry.

After a brief introduction (Chapter 1), highlights are given for the synthesis of isocyanates (Chapter 2), carbamates and ureas (Chapter 3), amines, imines, azo derivatives, and other noncyclic compounds (Chapter 4), and heterocycles (Chapter 5). A thorough summary of the kinetic and mechanistic studies is included in Chapter 6. Over the past decade and a half, the authors have published extensively on their own research in this field and are two of the leading authorities in this area. This book will be a useful addition to the library of researchers working in this area. It also represents an excellent starting point for someone interested in developing a program in catalytic carbonylations.

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JA975571E

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Structure and Properties of Rubberlike Networks. By Burak Erman (Bogazici University) and James E. Mark (University of Cincinnati). Oxford University Press: New York. 1997. xiii + 370 pp. $70.00. ISBN 0-19-508237-0.

Both Erman and Mark are well-known for their research contributions to rubberlike elasticity, and they have brought that experience to the preparation of this work to review a wide range of topics on the subject. This book covers much the same subject matter as their earlier introductory work, *Rubberlike Elasticity: A Molecular Primer*, Wiley, 1988, but at a much more comprehensive level, and does so in a readable, concise style. The authors limit their scope to equilibrium properties throughout, eschewing much discussion of viscoelastic behavior as a subject still too much in progress to be within their scope. The initial chapters of the new book present models for the equilibrium elasticity of network polymers in sufficient detail for the reader to comprehend the development of the field from its earliest days through recent treatments, with citations to much of the relevant original literature. The four chapters comprising this presentation will be a valuable resource, both to the scholar new to the subject and to those with some experience in the field. The models presented are applied in subsequent chapters to the discussion of several experiments, including the stress−strain behavior of network polymers, the swelling of networks, critical phenomena and phase transition in gels (i.e., in highly swollen networks), and thermoelasticity. Developments in numerical simulation of network elasticity are discussed, as are issues of segmental orientation in a strongly deformed network, the use of small-angle neutron scattering to study the chain structure in a network under deformation, and the preparation of model network polymers. These chapters provide useful, concise surveys of the literature on these diverse subjects. An additional four chapters deal with specialized topics, at various levels of development. These include networks from semiflexible chains, networks with complex distributions for the lengths of the chains between cross-links, networks comprising biopolymers, and networks filled with rigid particles. Each of these will be useful entries to the field, and are well documented. The authors emphasize the disparity between the strong technological importance and the relative lack of theoretical treatments available for filled elastomers. Finally, the authors have included an eclectic set of appendices, and a general bibliography to augment the literature cited at the end of each chapter. Each entry in the bibliography is annotated with a comment on the relation of the content to rubberlike elasticity.

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JA9756681

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Modern Catalytic Methods for Organic Synthesis with Diazo Compounds from Cyclopropanes to Ylides. By Michael P. Doyle. Wiley: New York. 1998. v + 652 pp. $69.95. ISBN 0-471-13556-9.

This book is a worthy addition to the experimentalist's library with some caveats. The authors have reviewed the, primarily English language, literature covered by the title. They have primarily concentrated on literature which has appeared since 1980. There has been considerable growth in the area since the recognition of the utility of employing chiral ligands to gain enantiomeric excesses and the employing of catalysts based on metals other than copper as a result of the work of Aratani with chiral copper(II) salicylimine systems and that with ruthenium by Robert Paulissen and Andre Hubert at Liege. An earlier treatise of metal salt catalyzed carbenoid reactions published in 1980 does exist. Users are cautioned to employ *Chemical Abstracts* back to 1900 to avoid repeating and reporting work which has already been accomplished.

The primary thrust is toward synthetic applications with numerous clearly presented reaction schemes, which include general conditions and tabulations of the impact of variation. They have included a number of specific experimental procedures which have been interleaved within the text and reaction schemes. Their number is perhaps excessive and occupies considerable space.

There are some mechanistic treatments. Sadly the present treatise is uncritical and repeats a number of simplistic proposals. Some of the mechanisms advanced were originally put forth by workers other than those cited.

Considerable attention is given to the question of the valence state of copper in diazo carbenoid reactions. It is not established, and the work cited to support Cu(I) is severely faulted. An uncited alternative interpretation and rebuttals have been published in full detail and include responses from the copper(I) proponent.

Each chapter ends with full references to the work cited, including titles, but there is no list of authors. The index is primarily one of compounds and at times becomes obscure due to employing acronyms for the multitudinous ligands employed to modify catalyst behavior. A glossary would have been most helpful for the intended users. If they knew what the acronyms meant, they probably would not need the book.

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