

## Computer Software Reviews

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**Electronic Conference on Trends in Organic Chemistry: ECTOC-1/CD-ROM. June 12–July 7, 1995.** Edited by Henry S. Rzepa, Christopher Leach, and Jonathan M. Goodman. The Royal Society of Chemistry: Cambridge, 1996. £50.00. ISBN 0-85404-8995.

This volume contains the entire record of the Electronic Conference on Trends in Organic Chemistry, held over the World Wide Web June 12–July 7, 1995. The CD-ROM is not a proceedings in the usual sense but rather contains the entire record of the meeting, including the keynote papers, papers, posters, and even the discussion that was carried out over the network. Also included are those articles that were originally served by the authors rather than being mounted on the official conference server. The CD-ROM is an exact copy of the WWW version, “warts” and all; i.e., even the rare corrupted or truncated image or structure file persists.

Using the CD-ROM is even more convenient than visiting the internet site (which is scheduled to disappear soon), as there are no delays due to busy network lines. The CD-ROM allows one to perform the complete keyword searches of the presentations, which makes it easy to locate an article or a particular set of related articles. Links have been included that enable one to utilize more powerful external search engines in the web version of the conference. To get maximal benefit from the graphics and other special features that have been included with many of the presentations (e.g., visualization of 2D and 3D information), several programs have been included with the CD-ROM with installation instructions.

All that one needs to make use of this interesting resource is a personal computer (Macintosh, MS Windows 3.1, or MS Windows 95) with a CD-ROM player and a World-Wide Web client such as Netscape. An internet connection is not required, although some documents have hyperlinks to optional supplemental sources of information that require full web access. Macintosh users can even use a WWW client included on the CD-ROM to view the local files. No computer expertise is required; getting started is as easy as opening a book. One simply points and clicks and is immediately in the center of the conference.

The printed documentation is concise and helpful to get started, except for the incorrect indication for MS Windows 3.1 users to start by double clicking on \$START.HTM. Double clicking on index.htm will work. Documentation related to the structure of the conference, necessary programs, optimal environment settings, how to perform a search, and announcements of future electronic conferences with appropriate links to external sites are included and explained in detail in files available on the CD-ROM.

The conference itself consisted of 77 papers on various aspects of organic chemistry, including synthesis, mechanisms, theory, and biological applications. The papers were peer reviewed and are of good quality. Thus, the CD-ROM contains a wealth of interesting information that is accessible in a convenient and efficient manner.

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## Book Reviews \*

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**Ullmann's Encyclopedia of Industrial Chemistry, Fifth, Completely Revised Edition, Volume A27: Thorium and Thorium Compounds to Vitamins.** Edited by Barbara Elvers and Stephen Hawkins. VCH: Weinheim. 1996. xv + 613 pp. \$650.00. ISBN 3-527-20127-0.

The fifth, completely revised edition of *Ullmann's Encyclopedia of Industrial Chemistry* is two encyclopedias in one. Divided into 36 volumes, the encyclopedia consists of an Alphabetically Ordered Series of 28 “A” volumes all containing articles on industrial chemicals, product groups, and production processes covering all aspects of the chemical and allied industries, together with the Basic Knowledge Series of 8 “B” volumes describing principles of chemical engineering, new and proven analytical methods, and the essentials of environmental protection technology. In addition, an updated Cumulative Index to both the A and B volumes is distributed annually. This encyclopedia is designed to provide the reader with a clear sense of orientation and rapid access to a wealth of information. Each article features consistent organization, an introductory table of contents, an extensive set of headings, and well-designed illustrations, formulas, and tables.

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**Advances in Oxygenated Processes. Volume 4.** Edited by Alfons L. Baumstark (Georgia State University). JAI Press, Inc.: Greenwich. 1995. x + 242 pp. \$97.50. ISBN 1-55938-451-4.

This book is the fourth in the series *Advances in Oxygenated Processes* edited by Alfons L. Baumstark. In continuation with the tradition and high standards of the earlier volumes, the subject matter here provides an in-depth coverage of important topics in “oxygen” chemistry in the organic, bioorganic, and biochemical areas. This volume consists of seven chapters, each covering distinctly different but related topics by authors who have made significant contributions in the field. A notable aspect of this volume is the inclusion of a chapter containing the general theoretical background on the electronic properties of singlet and triplet oxygen, including quantum theoretical calculations on several aspects of oxygen-addition reactions.

As appropriate, the book opens with Chapter 1 which contains the above-mentioned theoretical material, taking specific examples from S- and P-oxidation by singlet oxygen. The author, Frank Jensen, provides a very concise account of the electronic states of the oxygen molecule, emphasizing the possible reason why singlet and triplet oxygen react so differently with different reaction centers, simple facts such as why the former is electrophilic, and how the LUMO of the reaction center plays a key role in the geometry of the transition states as well as the final compounds. He also explains why theoretical insight is important for understanding the mechanistic details of addition reactions of singlet oxygen to many sites (in particular, S- and P-centers): it is hard to detect any of the proposed reaction intermediates; hence, there is little or no direct experimental data on the species involved in the reaction pathways. He thus reviews the various quantum theoretical models that are in current usage, explaining the underlying approximations in the various models and basis sets used, which in itself is highly useful to the general reader. The chapter ends with summary of the results from the various computational studies, predicting the structures of some as-yet unobserved intermediates.

Chapter 2, by Edward Clennan, reviews the theoretical and experimental data on sulfide photooxidation. The focus here is on the mechanism of dialkyl and alkyl aryl sulfide photooxidation of other sulfides (earlier reviews listed). The choice is made because although the photooxidation of dialkyl sulfides was the first such reaction reported (Schenck and Krauch, 1962), the overall mechanistic details are still not well understood. The chapter contains a listing of important rate constants, activation parameters and steric factors, NMR product yields, and relative trapping efficiencies for various quenchers in common use in such studies. These data are compared with the results of quantum theoretical calculations at various levels of approximation. The discussion at the end indicates the utility of parallel theoretical and experimental (e.g., NMR) studies of a given reaction.

Chapter 3 by Lazaro Cafferata and Jorge Furlong discusses in detail the thermal chemistry of tetroxanes, including preparative details of these unusual compounds. Their major objective is to provide a comparative analysis of the kinetics data and the mechanism of the thermal decomposition of a series of substituted 1,2,4,5-tetroxanes. On the basis of detailed analyses of the kinetic data, including solvation effects, it is concluded that the reaction mechanism involves the participation of free radicals, initially biradicals, analogous to the case for cyclic peroxides, such as 1,2-dioxetanes but different from those

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\*Unsigned book reviews are by the Book Review Editor.

in the thermolysis of 1,2-dioxolanes. Additional unanswered questions are posed at the end, which should be of particular interest to those in this area. Chapters 4 and 6 by Baumstark and co-workers review the chemistry of N- and P-compounds, specifically azohydroperoxides and the reactions of phosphorus compounds with 1,2-dioxetanes and 1,2-dioxolanes, respectively, the latter as a sequel to Chapter 3.

Finally, Chapters 5 and 6 deal with some rather applied aspects, oxidation in the paper industry. In Chapter 5 Sergi Sevchenko provides an in-depth account of the basic aspects of the biochemistry of lignin and its biosynthesis and biodegradation mechanisms. He points out that this chemistry is rich in mechanistic details, as exemplified by the fact that the oxidation of lignin in aqueous alkali solution is a combination of autocatalytic reactions, which result in the development of oscillatory processes. It is also found that oxygenated free radicals play a significant role in the oxidation of wood, although the underlying mechanisms remain to be established. In Chapter 6, Arthur Ragauskas presents additional interesting facets of the paper and pulp industry, focusing on bleaching via dioxirane chemistry, and ending with a brief discussion of some future directions in this field.

This volume thus covers a wide range of topics in oxidation processes in both depth and breadth, and should thus prove to be a valuable aid to both the starters as well as the advanced in the field of oxygen chemistry.

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#### **Active Metals: Preparation, Characterization, Applications.**

Edited by Alois Fürstner (Max Planck Institut für Kohlenforschung). VCH: New York. 1995. xviii + 464 pp. \$155.00. ISBN 3-527-29207-1.

*Active Metals* is a timely and interesting volume, one that reveals a strong and, to my mind, quite successful editorial perspective. In this book, Alois Fürstner has integrated two nominally disparate topics: recent advances in synthetic organic chemistry using activated metals and modern approaches to the preparation of novel activated metal systems. While this pairing might be interpreted cynically as a marketing ploy, my own response is considerably more generous. The book's page allotment is divided more or less equally between the two areas of research, with each chapter contributed by one or more of the principals in the development of the area.

The first five chapters and the organizationally misplaced Chapter 10 are focused on the organic chemistry of physically and chemically activated metals. Chapter 1, written by Reuben Rieke and several recent co-workers, covers the preparation and applications of Rieke metals, including magnesium, calcium, strontium, barium, zinc, aluminum, indium, nickel, and various forms of copper. Although methodology for the generation of the active metals is presented in significant detail, the emphasis remains on the reactivity and applications in the synthetic context. Chapter 2, covering the preparation and synthetic applications of allylic barium reagents, was written by Akira Yanagisawa and Hisashi Yamamoto. The third chapter, on the various low-valent titanium coupling processes collectively known as McMurry reactions, was written by Thomas Leckta, a relatively recent graduate of McMurry's program. Jean-Louis Luche and Pedro Cintas review ultrasound-induced activation of metals (Chapter 4), touching only briefly on the physicochemical effects of ultrasound (which have been more than adequately reviewed in recent years) before focusing on the use of sonochemically activated metals to effect electron transfer reductions and other reactions of organic substrates. A review by Paul Knochel covers the preparation and applications of functionalized organozinc reagents, including organozinc transformations catalyzed

or mediated by copper, palladium, and titanium (Chapter 5). The overlap between parts of this chapter and the organozinc sections of Rieke's review provides some interesting counterpoint. In Chapter 10, Fürstner himself provides an overview of recent advances in the use of supported metal systems (*e.g.*, Na/Al<sub>2</sub>O<sub>3</sub>, C<sub>8</sub>K, Ti-graphite, etc.), strongly emphasizing applications to organic synthesis.

The remaining chapters are devoted to a more inorganic perspective on the physical and chemical activation of metals, beginning with a review by Kenneth Klabunde and Galo Cardenas-Trivino on metal atom/vapor approaches to the synthesis of active metal clusters and particles composed of one or more metal elements (Chapter 6). This chapter also reviews several applications of these highly reactive materials to the formation of organometallic compounds, metal hydrides, and metal carbides. Chapter 7 is a limited review by Manfred Reetz and co-workers, covering this group's efforts to control the particle size and properties of transition metal clusters using electroreductive methods in conjunction with templating alkylammonium and phosphonium salts. In Chapter 8, Aleandri and Bogdanović review the use of magnesium anthracenide-tetrahydrofuran in the preparation of soluble magnesium metal and magnesium hydride, active powders of other metals, and a range of organometallic and intermetallic compounds. The use of these materials in organic, organometallic, and inorganic synthesis is also covered. Helmut Bönemann and Werner Brijoux review the preparation of nanoscale metal colloids, powders, and alloys by the chemical reduction of metal salts in the presence of stabilizing donors or surfactants (Chapter 9), providing the broader context in which the electrochemical work of Reetz is best evaluated. In Chapter 11, Ferdinand Hofer provides a critical summary of the physical/structural investigations of graphite-supported metal systems, complementing Fürstner's convincing review on the synthetic utility of these materials.

Although varying somewhat from chapter to chapter, the reviews are generally current, with some of the volume's more than 1300 references extending significantly into the 1995 literature. In pleasant contrast to many recent offerings, the book is extensively (16 pages) indexed. Most of the offerings are logically organized and reasonably well-written, although the clarity within the multi-authored chapter on Rieke metals, for example, is quite variable.

That the two parts of this book and the reviews within each part function synergistically is a tribute to Fürstner's insightful editorial control. While many will look no further than the topics obviously relevant to their own agenda, serious researchers on both sides of the fence will find substantial stimulation in "crossing over". The inorganic/materials chapters offer a multitude of unrecognized and unexploited possibilities for refinement and control in organic and organometallic synthesis; the organic chapters reveal much about what synthetic chemists can and cannot yet do.

Continuing a recent trend that should be further encouraged, most chapters generously provide experimental procedures for critical preparations and each review is written with a particular emphasis on technical detail and valuable "between the lines" comparative analysis. This informal, sometimes conversational, style reveals many procedural subtleties, and the discussion makes it possible even for novices in heterogeneous (or "near heterogeneous") preparative chemistry to exercise reasonable judgment in reproducing or extending these procedures. This is abundantly true, for example, in the highly informative chapter on the McMurry reaction, which was clearly written by someone who has spent considerable time "in the trenches".

This outstanding contribution belongs in more personal and graduate student libraries than the very high list price will ever allow.

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