

## Additions and Corrections

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**Search for a General Route to Metallaboranes via the Reaction of Monocyclopentadienyl Metal Chlorides with Monoborane. Synthesis and Reactivity of the Rhodaborane *nido*-1-Cl-2,3- $\{(\eta^5\text{-C}_5\text{Me}_5)\text{Rh}\}_2\text{B}_3\text{H}_6$**  [J. Am. Chem. Soc. 1998, 120, 2686–2687]. XINJIAN LEI, MAOYU SHANG, AND THOMAS P. FEHLNER\*

Page 2686: The cluster 2-(Cp\*Os)-3- $\{(\text{PPh}_3)_2(\text{CO})\text{Rh}\}\text{B}_3\text{H}_7$  should be 2-(Cp\*Ir)-3- $\{(\text{PPh}_3)_2(\text{CO})\text{Os}\}\text{B}_3\text{H}_7$ . We thank Prof. Lawrence Barton for bringing this error to our attention.

JA9855139

S0002-7863(98)05513-X

Published on Web 07/08/1998

## Computer Software Reviews

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**Comprehensive Organic Transformations on CD-ROM. A Guide to Functional Group Preparations.** By Richard Larock (Iowa State University). John Wiley & Sons, 1 Wiley Dr., Somerset, NJ. Phone: 1-800-225-5945. E-mail: custserv@wiley.com. List price \$125.00. (For comparison the book, *Comprehensive Organic Transformations*, lists for \$ 84.50.) ISBN 0-471-18649-X.

The COT CD-ROM is the electronic version of Richard Larock's popular book by the same title. The same CD-ROM runs on either Macintosh or Windows platforms and is provided as a Folio VIEWS Infobase. For IBM compatibles a 486 or faster computer is recommended with at least 4 MB of RAM, a CD-ROM drive, a VGA video card, and at least 4 MB of free disk space. Microsoft Windows version 3.1 or higher is required. Macintosh computers must have at least a 68020 processor with 4 MB of RAM, system 6 or higher, a CD-ROM drive, and 5 MB of free disk space. The CD-ROM was evaluated on a PowerMac 8500/120 with a 1.9 GB system disk and 64 MB of RAM.

The CD-ROM can be loaded onto your hard disk in two versions: the complete database or just the search program and indices. The small version requires 8.4 MB of disk space and must be used with the CD-ROM present in the drive. The large version requires 61.4 MB of space but can be used without the CD-ROM. Neither version is copy protected. Both the large and small versions are reasonably responsive running on the test system. One can get started without reading the manual, but the interface is complex, and reading the manual for 30 min is helpful. With practice one can easily navigate through the text. The quick-start instructions are reproduced in the software, and there is an extensive help menu.

*Comprehensive Organic Transformations* is Richard Larock's compilation of preparative organic reactions first published in 1989. The contents are arranged according to product functional groups. Over the years my students and I have found Larock's book to be a very useful guide to the literature. COT is a book that is really a database and could be very useful in electronic form, so I was intrigued when the CD-ROM version was announced. The *Comprehensive Organic Transformations* on CD-ROM is an electronic version of the book, rather than an electronic version of the underlying database. It has several useful features not present in the book, but is not as powerful as the same information would be if organized in a good database program.

There are several different ways to use the electronic book. Opening the document leads to six options: Getting Started, Transformation Index by Product, Transformation Index by Starting Material, Overview of Functional Groups and Reactions, Abbreviations and Synonyms, and Browse *Comprehensive Organic Transformations*. The final option displays the complete text of the book. The transformation indices present lists of starting materials and products. Double clicking on any line moves you to the appropriate place in the main text.

More interesting options are found under the search menu. The text can be searched by Transformations (From:To), Transformations by

Products, Transformations by Starting Materials, Book Headings, Journals, Reagents, and Personal Information. The Folio VIEWS program is a text database, and there are no provisions for structure searches. The transformations (From:To) searching is a real disappointment. Say you are interested in how to convert an alkene into an alcohol. When you enter "from: alkene to: alcohol", you get no hits. For each line in the search it gives you the number of qualified hits—a very nice feature. Under alcohol there are only 12 hits, so it is clearly the wrong name. To use the book or CD effectively, you need to learn how Larock names compounds. Searching "from: alkene to: ol" turns up 304 hits, which include useful transformations such as hydroboration. The search also turns up many useless hits such as a nickel-catalyzed addition of Grignard reagents to alkynes. This particular entry has 14 different transformations with "alkene" present in some of the starting materials and "ol" present in some of the products. None of the "alkene" starting materials lead to "ol" products, so this is a false hit. Unfortunately the search program is set up so that any "alkene" in the starting material list will match any "ol" in the product list. This search strategy produces so many false hits that it is next to useless. Transformation searching by product or starting material is not marred by false hits, but it is not a very precise strategy and leads to long lists of entries. In practice, just browsing the Transformation Index by Product list and clicking on the transformation of interest is as convenient as the searching functions.

When looking for specific transformations, a student using the book found the desired information more rapidly than one using the CD-ROM every time. In searching the book one can go to the appropriate product chapter in the table of contents and browse. Using the transformations searches efficiently requires a very precise understanding of the compound nomenclature. With more experience using the CD-ROM, one's efficiency would certainly improve, but greater efficiency also could be expected with regular use of the book.

In contrast, reagent searching is a very useful function. Searching "Bu3SnH" turns up 87 hits that can be sequentially displayed by clicking a button. Using this feature you can find every reaction using NiBr<sub>2</sub> as a catalyst or reagent in less than a minute. Wildcard characters can be used in the searches. A general query will also let you do complete text searching and identify every occurrence of a word in the book. There are 48 entries with "Lewis", and they can be displayed in sequence. Searches of this type are just not feasible using the book.

The electronic interface has a number of features. Text can be highlighted and bookmarks added for easy retrieval. Notes can be added to the book, and the note text is searchable. Different entries can be connected by links to facilitate moving from one entry to another. All of these modifications can be saved. Any entry, including graphical entries, can be selected and printed. Neither text nor graphics can be copied or exported.

Although the accompanying literature suggests that a few new entries have been added, the coverage of the literature is essentially identical

to that of the original book and is current through 1987. Updates may become available in the future.

Comprehensive Organic Transformations on CD-ROM is an electronic book rather than an electronic database. The single most useful feature is reagent searching. It is not set up to do structure searching, and the transformation (From:To) searches are flawed by an organizational scheme that leads to many false hits. The content is nearly identical to the book, and the cost is half-again as much. For general

browsing I do not see that the electronic version offers advantages over the book. I would recommend the CD-ROM version on the basis of its reagent searching feature.

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JA9759120

S0002-7863(97)05912-X

## Book Reviews

**Nonionic Surfactants: Organic Chemistry. Surfactant Science Series. Volume 72.** Edited by Nico M. Van Os (Shell International Chemicals B.V.). Marcel Dekker, Inc.: New York, Basel, Hong Kong. 1998. xiv + 291 pp. \$145.00. ISBN 0-8247-9997-6

This monograph, edited by the late Nico van Os, gives a focused account of the organic chemistry, especially the synthesis, of nonionic surfactants. The chapters are laid out in a consistent manner, and roughly arranged in order of importance to the detergent industry. The contributions are proficiently written by experts in the field, all of whom have industrial affiliations. Reference material is very extensive and generally up to date. Unfortunately, the accessibility of the book is marred somewhat by a poor index.

Since most nonionic surfactants in use are of the polyoxyethylene (POE) type, it is fitting that the first chapter deals with the chemistry of the POE chain. The remaining eight chapters each address a separate type of surfactant, extending beyond what may be considered "organic chemistry". All do, in fact, make excursions into the physical properties, applications, and environmental issues pertinent to the surfactants in question. Chapter 1, written by Charles L. Edwards, emphasizes the factors affecting the POE chain length, and gives an excellent account of polymerization catalysts. In the second chapter, Robert M. Weinheimer and Pierre T. Varineau cover POE alkylphenols, presenting a brief treatment of manufacture, and a comprehensive discussion of product composition. The authors manage to convey a great deal of information by the inclusion of 33 tables in this section. The third chapter, also written by C. L. Edwards, takes a similar approach to POE alcohols. In this treatment, the emphasis is more on synthesis and preparation, and less on properties and applications. A useful breakdown of the physical properties of a large number of commercial products is, however, presented. In the following chapter on POE esters, Kurt Kosswig covers the material in a similar manner, with only brief attention given to nonproduction aspects such as toxicology and biodegradation. Chapter 5, once again written by C. L. Edwards, deals with POE mercaptans. In keeping with the lesser importance of this class of surfactants, this is a short treatment that briefly describes the salient points of synthesis, properties, and applications of these compounds. Chapter 6, on POE alkylamines, is written by Michael D. Hoey and James F. Gadberry and is still more condensed. Most emphasis is placed on synthetic aspects of these quasi-ionic surfactants. In Chapter 7, Anna Lif and Martin Hellsten describe nonionic surfactant containing the amide group. Their treatment is somewhat more extensive than that of the previous two chapters, especially with regard to surfactants containing both amide and carbohydrate groups. Chapter 8, by Jeremy Lewis, deals with polyol ester surfactants. It gives a detailed account of these compounds, separately describing glycol, glycerol, polyglycerol, sorbitan, sucrose, and polyoxyalkylene polyol esters. Last but not least, Ansgar Behler, Karlheinz Hill, Andreas Kusch, Stefan Podubrin, Hans-Christian Raths, and Günther Uphues discuss nonionics as intermediates for ionic surfactants. They deal with the conversion of POE surfactants to various ionic adducts, including sulfates, sulfonates, phosphates, carboxylates, and quaternary ammonium compounds. The emphasis is on preparation, with a fair dose of properties, toxicology, and analysis added. The material is especially exhaustively referenced.

The usefulness of this monograph is greatly enhanced by its emphasis on existing commercial detergent products, including trade names,

manufacturers, and country or origin. It is a well-conceived and well-executed piece of work, which deserves high recommendation.

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JA975700R

S0002-7863(97)05700-4

**Bioinorganic Chemistry: Trace Element Evolution from Anaerobes to Aerobes. Structure and Bonding Series, #91.** Edited by R. J. P. Williams. Springer: Heidelberg. 1988. 207 pp. ISBN 3-540-63548-3.

The volume contains four chapters, Biological Nickel by J. C. Fontecilla-Camps, Nickel in  $F_{430}$  by J. Telsler, Heme proteins in Anaerobes by I. A. C. Pereira, M. Teixeira, and A. V. Xavier, and Evolutionary Aspects of Copper Building Centers in Copper Proteins by B. Abolmaali, H. V. Taylor, and U. Weser. Dealing with proteins containing the elements nickel, iron, and copper, the volume elaborates on the notion that evolutionary expediency led to the prevalence of nickel proteins in anaerobes whereas copper was exploited by aerobic organisms. Iron-containing proteins span both classes. The first chapter deals mainly with the nickel-containing proteins urease, hydrogenase, and carbon monoxide dehydrogenase (CODH). Included are the proposed or real metal-building sites of the proteins and a discussion of the mechanisms of enzyme action. This chapter represents a useful summary of the current views of the subject. The following chapter, on  $F_{430}$ , deals with the structure and physical properties of the macrocyclic nickel building site which is involved in the conversion of carbon dioxide to methane. Included is a discussion of the role of the macrocyclic ligand in controlling the oxidation state changes of the nickel atom. The chapter on heme proteins may have less appeal to inorganic chemists because the approach to the subject is more biochemical than chemical. This is perhaps because the heme proteins appear to serve as redox reagents. The final chapter, dealing with the evolution of copper proteins and the structures and functions of most of the known copper proteins is probably the most stimulating. Inorganic chemists interested in biological copper should read this chapter. It contains a description of how the earth's early harsh environment led to the adaptation of certain metalloproteins. As a more oxygen-rich atmosphere developed, various new metalloproteins began to appear in order to take advantage of the dioxygen. In particular, an extensive variety of copper proteins evolved, most of which are involved directly or indirectly with reactions of dioxygen. The chapter provides a comprehensive survey of copper proteins. It includes the known structures of the proteins and their functions. An inorganic chemist will find a fascinating variety of unusual structures and chemical transformations.

Aside from the intrinsic interest in the metalloproteins described here, the potential for developing new, important, practical catalysts by taking clues from biology is one of major goals in understanding the mechanisms of the biological systems. The present volume provides a useful summary of how biology has employed common transition metals in a number of intriguing catalytic transformations.

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JA9856147

S0002-7863(98)05614-5