Additions and Corrections

Encyclopedia of Analytical Chemistry. Applications, Theory and Instrumentation [*J. Am. Chem. Soc.* **2001**, *123*, 3621].

The number of pages and the price listing for this 15 volume encyclopedia were erroneously reported. The accurate number of pages is 13 970, and the current price is $6000.00.

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Computer Software Reviews

IUPAC Name Pro 4.5 with Name to Structure Module. Advanced Chemistry Development, 133 Richmond Street West, Suite 605, Toronto, Ontario M5H 2L3, Canada. http://www.acdlabs.com. Industry price $3900.00; academic price $995.00.

IUPAC Name Pro 4.5 software is designed to generate systematic names for general organic compounds on the basis of the guidelines specified by the International Union of Pure and Applied Chemistry (IUPAC). The program can accommodate all elements and metal cations, except noble gas elements. The pre-release, stand-alone version for MS Windows that was reviewed came as a CD-ROM and was easily installed on an IBM-compatible PC (Pentium 4000 processor).

Entry into the naming program is through the ACD/ChemSketch interface, which is a user-friendly chemical drawing program. A user who is familiar with such programs can easily draw a structure in ChemSketch and generate an IUPAC name for the compound using the “Name” button at the bottom of the screen. A User Guide is available as a printable, electronic file, but reference to it was not necessary to use the program. In fact, the user manual provided with this software was for an older version, namely for Name Pro 4.0. Instructions for use can also be obtained from the ACD Web site.

The program quickly generated accurate systematic IUPAC names for many types of organic compounds. A useful feature in the name window is the option to view the protocol used to name a compound. When this option is selected, the protocol appears on the right side of the screen along with hyperlinks to specific IUPAC rules used to name that compound. There are limitations to the types of compounds that the program can tackle, however. For example, complex bridged systems and spiro compounds containing polycyclic components are not supported. In such cases, an error message will inform the user that the molecular structure cannot be named. The user has the option to set a maximum limit for the time that the program will expend in attempting to name a compound; if this time limit is exceeded, an error message will prompt the user of the failed attempt.

Name Pro 4.5 can accommodate double bond geometry and stereogenic centers at carbon atoms. Other types of chirality, such as axial, planar, helical, and relative stereochemical descriptors, such as syn/anti, endo/exo, and R*/S*, are not supported. The algorithm utilizes a depth of comparison of up to 10 ligands in determining the absolute configuration of a chiral center. Stereobonds must be drawn according to convention for accurate assignment of configuration. The user manual contained clear descriptions of these conventions and ways to use the preference tools optimally.

The program is capable of naming steroids, alkaloids, terpenes, most carbohydrate derivatives, and some amino acid derivatives on the basis of the parent natural products. The tested version of the program recognizes nearly 130 basic tricyclic and greater parent structures of natural products.

Name to Structure capability was available in the tested version of the software; however, this module was of limited utility. Exact IUPAC or natural product-derived names for organic compounds must be provided to obtain reliable structures.

The software can also generate names for a list of structures (up to 99) contained within a Standard Data File (SDF). A sample SDF was available to test this feature, and instructions on how to prepare an SDF for a list of structures is given in the user manual. This feature will be useful in naming multiple compounds that constitute libraries generated by high-throughput synthesis methods.

In summary, ACD/Name Pro 4.5 software is a useful tool for quickly generating IUPAC names for most organic compounds. The capability to generate names for multiple compounds in a batch mode will find applications in the high-throughput synthesis area. However, the user must be aware that certain complex structural features are still not accommodated by this version of the software.

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Book Reviews

Organic Synthesis on Solid Phase. Supports, Linkers, Reactions. By Florencio Zaragoza Dörwald (Novo Nordisk A/S MedChem Research, Malov, Denmark). Wiley-VCH: Weinheim. 2000. xx + 474 pp. DM 268 (approximately $125.00). ISBN 3-527-29950-5.

There is suddenly a myriad of edited books, practical guides, and other monographs available on combinatorial chemistry and solid-phase organic synthesis. Obviously, it is becoming more and more challenging for new books to distinguish themselves and offer new features of broad interest to the chemical community. This new one by F. Z. Dörwald succeeds admirably. The aim of the book, as stated by the author, is to give the reader a well-structured and exhaustive collection of synthetic procedures that can be realized on insoluble supports. The only other practical handbook of this sort is *The Combinatorial Index*, by Barry A. Bunin, published in 1998. Being more recent, *Organic Synthesis on Solid Phase* is more up-to-date but also is a more comprehensive text.

Most types of chemical transformations, including cycloadditions, redox processes, organometallic reactions, and several other transformations, have now been carried out on solid support. Yet, in the planning of such efforts, all practitioners of solid-phase organic synthesis recognize the potential savings in time and effort gained by referring to examples of prior work that discuss the feasibility of the desired reactions. Indeed, with so many new variables, such as the type and characteristics of resins and linkers and the consequent limitations on solvent and other reaction parameters, experimental conditions known to work well in solution-phase chemistry are seldom entirely transferable to solid-supported synthesis. This book, by providing access to a comprehensive source of very up-to-date references (the total number of references is over 2500), serves as a very useful compendium of solid-phase synthetic procedures. The accompanying text is very informative, highlighting key theoretical aspects on each type of reaction while guiding the reader through the tables and figures.

The book starts with three introductory chapters on the general aspects of solid-phase organic chemistry: synthetic techniques and analytical tools, supports, and linkers, respectively. These chapters are supported by a wealth of figures and tables. Featuring almost 100 pages with more than 600 references, the chapter on linkers is particularly useful; it describes more than 50 different classes of linkers according to the functional group they attach. An almost equal number of tables is included to illustrate many examples of loaded resins with cleavage conditions and final products (including yield and purity). The next 13 chapters are organized in a highly subdivided fashion by class of supported product made, namely: organometallic compounds, hydrocarbons, alkyl and aryl halides, alcohols and ethers, sulfur compounds, organoselenium compounds, nitrogen compounds, phosphorus compounds, aldehydes and ketones, carboxylic acid derivatives, carbonic acid derivatives, heterocycles, and oligomeric compounds. Although organization by class of product is convenient and generally more preferable, at times it may be desirable to browse such a handbook by the category of reactions or substrates. Fortunately, the book ends with a very detailed index that helps overcome this small limitation. For example, although there is no section on the popular Suzuki cross-coupling reaction, the index refers to several relevant sections of the book. A search on Suzuki cross-coupling reactions as a means to make alkyl-substituted derivatives will lead the reader to a section in Chapter 5 (“Preparation of Hydrocarbons”) entitled “Coupling Reactions with Boranes”. For applications of the same reaction in the preparation of biphenyl compounds, yet another section of Chapter 5, “Preparation of Biaryls”, must be consulted, although the latter blends other related processes, such as the Stille reaction.

Each section is filled with exhaustive tables showing the structures of starting and product resins, including the type of polymeric support, and accompanied with details on reaction conditions and the original literature references. The tables are not quite comprehensive, but additional relevant references are also compiled. Although readers will most likely consult the original sources before attempting a reaction, a small number of detailed procedures are provided for the most popular transformations.

Overall, this book is a very worthy addition, if not an essential one, to the library of all academic and industrial laboratories involved in solid-phase organic synthesis. It is the type of practical handbook that is bound to get worn out and exchange hands rapidly among labmates and colleagues.

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Introduction to Perturbation Theory in Quantum Mechanics. By Francisco M. Fernandez (University of La Plata, Argentina). CRC Press LLC: Boca Raton, FL. 2001. xii + 272 pp. $99.95. ISBN 0-8493-1877-7.

Perturbation theory provides analytical, approximate solutions for the Schrödinger equation in many simple but nontrivial problems arising in theoretical chemistry. These analytical solutions are often useful for physical interpretation and suitable for numerical calculations. Unfortunately, the standard textbook formulas for high-order perturbation corrections are often unmanageable. This book shows several alternative strategies that are easily programmable. Since the use of computer algebra is mandatory for high perturbation orders, the Maple package is extensively used throughout the book to derive formulas and create tables. Texts for all Maple programs used in the book are collected in the supplement, so that the reader can reproduce and modify the formulas.

The book consists of nine chapters, which focus mainly on perturbation theory for bound stationary states. Chapter 1 lists the basic ideas and matrix equations of perturbation theory in number representation and illustrates their application on one-dimensional harmonic and anharmonic oscillators. Time-dependent perturbation theory is also outlined here. Chapter 2 deals with alternative coordinate representation, leading to inhomogeneous differential equations, and describes three widely used strategies to solve them (one of which was originally developed by the author). These strategies are also applied to the anharmonic oscillator problem and the Zeeman effect on the hydrogen atom. Chapter 3 describes three approaches that allow bypassing the explicit treatment of the wave function, and Chapter 4 applies the methods developed in the previous chapters to the treatment of the Stark and Zeeman effects on hydrogen atoms and molecular ions. Chapter 5 is dedicated to the Schrödinger equation with Dirichlet and periodic boundary conditions. Problems of this sort are useful in the theory of solids, molecular interactions, quantum wells, rotation spectra, etc. The convergence rate of the perturbation series is covered in Chapter 6, which also describes some methods for the summation of divergent series. Chapter 7 reviews the particular form of perturbation theory that is based on the expansion of the potential energy function in the Taylor series about a conveniently chosen coordinate point. In Chapter 8, the approaches developed for boundary states are applied to scattering states, and in Chapter 9, they are applied to problems in classical mechanics.

This book summarizes in detail a wide variety of techniques used in perturbation theory that were developed for particular problems. To make the methods easily comparable, they are applied to the same models. Some of these models have exact solutions, so that improvements in the perturbation series and their limitations become clear. The author intentionally avoids problems that require numerical computation and tries to keep the mathematics as simple as possible in order to concentrate the reader’s attention on the ideas underlying each method. For those interested in probing the subject further, extensive bibliographic references are provided. Overall, the book offers an invaluable source of ideas for theoreticians applying perturbation methods to various problems in chemistry and physics; it can also be used for teaching undergraduate and graduate courses in this subject.

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Modern Carbonyl Chemistry. Edited by Junzo Otera (Okayama University of Science). Wiley-VCH: Weinheim. 2000. xx + 614 pp. $169.95. ISBN 3-527-29871-1.

Modern synthetic organic chemistry relies heavily on the transformations associated with the carbonyl group. In *Modern Carbonyl Chemistry*, Otera’s assembly of reviews by prominent scholars successfully presents a stimulating overview of the important concepts, recent developments, and classic reactions of carbonyl chemistry. One of the helpful strategies utilized in the text is a reliance on specific examples to illustrate key points as well as the historical developments and milestones achieved in each area. Additionally, the X-ray crystallographic data, transition-state structures, mechanisms, and conformational analyses that appear throughout render the concepts accessible to those less familiar with the material and provide a context for advanced readers wishing to extrapolate to new systems.

Several chapters that address the chemistry of Lewis acid−carbonyl complexes from theoretical and experimental perspectives establish a foundation for further discussions on carbonyl differentiation, recognition, chelation, and electrophilicity. The middle chapters, comprising over 40% of the book, highlight the venerable aldol and allylation reactions. This section offers a broad overview of well-established, practical modern methods and illustrates the application of these important reactions in the total synthesis of natural products. Additional chapters that concentrate on a spattering of more eclectic topics round out the material with discussions on acyllithiums, pinacol couplings, engineered catalysts, Michael-type additions, aqueous media, and radical reactions.

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