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BOOK REVIEWS

Modern Methods of Drug Discovery. Edited by Alexander Hillisch (EnTec GmbH) and Rolf Hilgenfeld (Institut für Molekulare Biotechnolgie e.V.). Birkhäuser Verlag: Basel, Boston, Berlin. 2003. x + 292 pp. $149.00. ISBN 3-7643-6081-X.

This is an excellent monograph that gives a broad overview of current and future methods that are and may be employed in the field of drug discovery. Because medicinal chemistry is a highly interdisciplinary subject, such a broad sweep of state-of-the-art practices in drug discovery should be beneficial to anyone interested in pharmaceuticals. The book should be especially useful to graduate students and practicing chemists who would like a better grasp of the process of drug discovery. It could also be used as a text for graduate students and perhaps for advanced undergraduates, particularly given the increasing interests in having undergraduates in chemistry learn more about medicinal chemistry.

The editors have done an outstanding job of bringing together a collection of timely reviews of topics that range from proteomics and bioinformatics to structure-based drug design and computer-based modeling methods. Based on my own experiences, the material presented is both accurate and current. Although each chapter can be read separately and out of order, the editors have made a good effort to refer the reader to other chapters where a particular subject is discussed. Many readers will enjoy the topics that blend experimental and theoretical approaches for lead discovery and optimization. I found the chapters that cover the role of protein 3D-structures in the drug discovery process and structure-based design of combinatorial libraries, 3D-QSAR, and computer-assisted predictions of toxicity and metabolism to be particularly enjoyable because of my own research interests. There are also discussions of physiochemical concepts and NMR-based screening as well as reviews of high-throughput screening and combinatorial chemistry.

In summary, this book would make an excellent addition to the library of those interested in the complex field of drug design and discovery. The coverage of material is remarkably close to those topics covered in the American Chemical Society's Continuing Education short course in computational chemistry and computer-assisted drug design and would make wonderful background reading. As the course director, I am tempted to recommend this book as essential material prior to taking this course.

J. Phillip Bowen, *University of Georgia*

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Kirk-Othmer Encyclopedia of Chemical Technology, Fifth Edition. Edited by Arza Seidel (John Wiley & Sons, Inc., Hoboken). John Wiley & Sons, Inc: Hoboken. 2004. $5400 for prepaid set or $6075 for standing order. Online pricing based on needs of user. ISBN (set): 0-471-48810-0.

This well-known encyclopedia brings together up-to-date information on chemical technology from "properties, manufacturing, and uses of chemicals and materials" to "emerging technologies, economic aspects, and environmental and health concerns". Some of the important topics that are covered in this set include design of chemical products, chemical warfare, chemoinformatics, combinatorial chemistry, fuel cells, fullerenes, green chemistry, hydrogen chemistry, indoor air pollution and control, ionic liquids, lithographic resists, metallocene catalysis, nanotechnology, and process system engineering. The 27 volumes will be published systematically over the next four years with volumes 1 and 2 being published in January, volumes 3 and 4 in March, and so on. An index and a supplement volume are included in the set, which is also available online.

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Electrokinetic Phenomena. Principles and Applications in Analytical Chemistry and Microchip Technology. Edited by Anurag S. Rathore (Amgen, Inc., Thousand Oaks, CA) and Andras Guttman (Diversa Corporation, San Diego, CA). Marcel Dekker: New York and Basel. 2004. xiv + 476 pp. $175.00. ISBN 0-8247-4306-7.

This book provides an excellent summary of contemporary electrophoretic techniques and methodologies currently in widespread use in analytical chemistry. It contains 15 chapters with each focusing on a particular aspect of electrophoresis, such as capillary isoelectric focusing and capillary electrochromatography. The chapters are written by one or several experts in the field who come from both academia and industry. Individually, they provide thorough, up-to-date, and well-referenced treatments of specialized topics. The early chapters emphasize more fundamental aspects of electrophoresis, whereas the latter ones deal with "cutting edge" subjects. The authors of Chapter 13, for example, discuss NMR detection in electrophoresis, which is still in its infancy.

As a whole, the book covers the topic of "electrophoresis as a separation method" very well. The book should be of considerable value to all investigators who use electrophoresis in their research or in the classroom, which represents a significant fraction of analytical, biophysical, and biochemists.

This reviewer does have two minor criticisms. First, I think a more accurate title of the book would be "Electrophoretic Phenomena" rather than "Electrokinetic Phenomena" because the former title is more specific. Electrokinetic phenomena, such

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as electric birefringence and the various electroviscous effects, were not treated in the book. Second, the unmentioned emphasis of the book is on electrophoresis *as a separation method*. Unquestionably, this has been its primary use and strength in the eyes of the majority of researchers. I would argue, however, that electrophoresis has more to offer. Electrophoretic mobilities themselves have the potential for providing direct information about macro-ion charge, size, interactions with other species, and, if present, interactions with the solid supporting medium. This subject, however, is almost entirely ignored in the book.

These criticisms aside, I think it is an excellent book that everyone who works in the field of electrophoresis will want to either own or have access too. It has my enthusiastic endorsement.

Stuart Allison, *Georgia State University*

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Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin, Volumes 1 and 2. Edited by Erkki J. Brändas (Uppsala University) and Eugene S. Kryachko (Bogoliubov Institute for Theoretical Physics, Kiev, and University of Leuven, Belgium). Kluwer Academic Publishers: Dordrecht. 2003. xxxii + 678 pp (Volume 1) and xxxii + 696 pp (Volume 2). $450.00 (set). ISBN: 1-4020-1286-1 (set).

In the Foreword, the editors note that "it is with respect and devotion that we point out Per-Olov Löwdin's pioneering and limitless efforts to found and establish the science of Quantum Chemistry. With his extraordinary capacity, Per-Olov Löwdin made basic contributions to the development, provided the conceptual framework and introduced fundamental concepts, and added rigor to the field."

Löwdin established the Uppsala Quantum Chemistry Group in 1955 and the Quantum Theory Project at the University of Florida in 1960. In addition to his seminal papers on fermion density matrices, perturbation theory, and the fundamentals of quantum and statistical mechanics, he organized many summer and winter schools, institutes, and symposia. His remarkable legacy includes the many students and postdoctoral associates who studied with him. He was the principal driving force behind the establishment of the *International Journal of Quantum Chemistry* and *Advances in Quantum Chemistry*.

Although space restrictions preclude even a brief review of each chapter, the first chapter of Volume 1 by Shull deserves special mention. His chapter opens with the statement that "Per-Olov Löwdin was a veritable giant in the scientific universe, a dynamo of energy, full of *joie de vivre*, and a kindly mentor to us all." Shull provides insight into Löwdin's life and his scientific influence by indicating how their lives were entwined. Löwdin received his doctorate in theoretical physics in Uppsala, Sweden in 1948, the same year Shull received his in physical chemistry at Berkeley. By chance they were roommates at the 1951 Shelter Island Conference on Long Island. Attendance at the conference was limited to 25 participants and was clearly an exciting and stimulating occasion with Mulliken, Lennard-Jones, and Coulson present. This chance meeting was the beginning of a long friendship that resulted in many scientific collaborations and the establishment of the famous summer schools in quantum chemistry.

Shull concludes his chapter with a poem written by his wife as her personal tribute to Löwdin. The poem, appropriately called, *The Swedish Doorman*, will likely resonate with his many friends and colleagues and with the thousands of scientists who attended his close to 70 summer schools and winter institutes in Sweden and Florida.

The 49 chapters of the two volumes are a fitting tribute to the legacy of one of the most important scientists of the 20th century. Most chapters highlight Löwdin's scientific contributions through his publications and his personal communications. Examples of his broad interests include, in no particular order, the correlation energy, the reduced density matrix, the charge and bond order matrix, natural orbitals and natural geminals, projectors and idempotency, N-representability, symmetry breaking, the pairing theorem, Sturmian basis functions, partitioning techniques, and, of course, Löwdin orthogonalization, Löwdin's path diagram, and Löwdin's symmetry dilemma. Late in his career, he became interested in a formal definition of the term *molecule* within quantum mechanics, the subject of a comprehensive chapter by Woolley and Sutcliffe. Like many chapters, this one deals with a fundamental topic of continuing interest.

This two-volume set will provide many hours of stimulating and engaging reading for serious students of quantum chemistry. It provides an anecdotal record of the development of the field, valuable insight into the current status of the discipline, and perhaps most importantly the context of some important problems that await the attention of future generations of researchers.

Russell J. Boyd, *Dalhousie University*

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