Book Review

An Introduction to Chemoinformatics By Andrew R. Leach (GlaxoSmithKline, Stevenage, U.K.) and Valerie J. Gillet (University of Sheffield, U.K.). Kluwer Academic Publishers: Dordrecht. 2003. xvi + 260 pp. $74.00. ISBN: 1-4020-1347-7.

Robert S. Pearlman

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BOOK REVIEWS

Mesoscale Phenomena in Fluid Systems. Edited by Fiona Case (Colgate Palmolive Company) and Paschalis Alexandridis (The State University of New York). American Chemical Society (distributed by Oxford University): Washington, DC. 2003. xiv + 447 pp. $185.00. ISBN: 0-8412-3867-7.

This book is based on the presentations given at the "Mesoscale Phenomena in Fluid Systems" symposium held during the 224th ACS National Meeting in Boston in 2002. It also contains some contributions from the related symposium "Nanoscale Organization by Self-Assembly" given at the 2002 ACS Division of Colloid and Surface Science meeting in Ann Arbor. Its 25 chapters are organized into the following three sections: Characterizing Mesoscale Structure and Phenomena, Predicting Mesoscale Structure and Phenomena, and Applications of Mesoscale Phenomena. An author and a subject index complete the book.

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Glow Discharge Optical Emission Spectroscopy: A Practical Guide. By Thomas Nelis (Ste Croix, France) and Richard Payling (The University of Newcastle, Australia). Royal Society of Chemistry: Cambridge. 2003. xii + 212 pp. $249.00. ISBN: 0-85404-521-X.

Nelis and Payling present here a very straightforward, informative bench guide for glow discharge optical emission spectroscopy (GD-OES). GD-OES is a technique that is rapidly growing in application because of its unique capabilities to provide rapid, sensitive depth profiles of diverse materials ranging from computer hard disks to automotive components. Both authors have a long history of working with GD-OES manufacturers as scientists and experts in development and applications. Payling has been a key participant in the workings of the European Community Thematic Network on Glow Discharge Spectroscopy for Spectrochemical Analysis and ISO Technical Committee TC-201, Surface Chemical Analysis.

The authors suggest in the preface that the text is a user's guide for laboratory managers and technicians to learn about the technique from a "hands-on perspective". The nuances of instrument operation are explained from a first-principles basis, providing the user with a fundamental rationale that is not found in a typical manual of operation. Aspects of optimizing instrument performance and of validation, choices of analytical standards, and quantification in both the concentration and depth regimes are described. Statistical methods of analysis are presented with regard to calibration as they are outlined in the ISO 9000 standard for quality management systems and ISO 10012-1 and 17025 relating to quality assurance in third-party analyses. GD-OES analyses are performed in three basic formats: bulk analysis, qualitative depth profiling, and compositional (quantitative) depth profiling. The authors take the user through the strategic and methodological approaches to achieve successful analyses. Chapters describing correction of drift and troubleshooting aid the analyst when difficulties arise. Throughout the book, the authors do an excellent job in not revealing biases toward or against any particular instrument manufacturers or particular methodologies.

What sets this book apart from a simple user's manual is the inclusion of demonstrative data taken from the literature to aid analysts in optimizing their own systems. The references are very relevant and up-to-date. Tables of typical and alternative analytical wavelengths are a very useful addition. Finally, in a quite novel approach, the underlying physics that govern source operation and performance is described in one of the last chapters of the book. Philosophically, this allows laboratory managers and technicians to get their bearings about the generation of good data without being bogged down in plasma physics.

All in all, the authors have produced a highly useful text that is a true service to the users of this technique. On the basis of the objectives set out in the preface, the book does indeed deliver the targeted outcomes. I would expect that it will be an essential reference in all laboratories in which GD-OES instruments are used and thus recommend it to all current users or those considering implementing the technique. N.B. Richard Payling died in a hiking accident in February 2004. His passing is not only a loss to his family, but to the GD-OES community as a whole. He was truly a gentleman and scholar.

R. Kenneth Marcus, *Clemson University*

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Advances in Chemical Physics. Volume 128 Edited by Stuart A. Rice (University of Chicago). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. x + 384 pp. $175.00. ISBN 0-471-44528-2.

Editor Stuart Rice is carrying on the fine tradition of the *Advances in Chemical Physics* series by assembling authoritative reviews spanning a diverse range of topics in modern physical chemistry. The topics in this volume include subjects in condensed phase and macromolecular chemistry, such as polymer crystallization (Muthukumar), constrained Brownian motion (Morse), and the dynamics of magnetic nanoparticle systems (Jönsson). For researchers interested in electronic structure and reaction dynamics, there are contributions on the momentum density perspective of electronic structure (Thakkar) and the wave packet theory of photodissociation and reactive scattering (Balint-Kurti).

The first half of the book is devoted to nucleation phenomena in crystallization of polymers and constrained Brownian motion, providing an excellent introduction into thermodynamic, statisti-

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cal mechanical, and kinetic treatments of macromolecular systems. These topics are of increasing interest because of potential biological applications. The chemical physics of magnetic nanoparticle systems will be of interest to a wide range of materials scientists and engineers because of their applications in magnetic storage. Balint-Kurti's presentation of calculations of the dynamics of wave packets is timely, given the current popularity of this approach to photodissociation and reactive scattering processes in increasingly complex systems. Representations of electronic structure by momentum density, while firmly based in experimental measurements such as Compton scattering and (e,2e) spectroscopy, have received relatively little attention in recent years. Thakkar's contribution may play a role in raising the profile of this perspective on electronic structure. This volume of *Advances in Chemical Physics* should be a valuable resource for graduate students and researchers interested in authoritative reviews of the subjects presented.

Robert E. Continetti, *University of California, San Diego*

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International Tables for Crystallography, Volume D: Physical Properties of Crystals. Edited by A. Authier (Université Pierre et Marie Curie). Published for the International Union of Crystallography by Kluwer Academic Publishers: Dordrecht, The Netherlands. 2003. xii + 522 pp. $220. ISBN: 1-4020-0714-0.

The aim of this volume, according to the editor, is "to provide an up-to-date account of the physical properties of crystals, with many useful tables, to a wide readership in the fields of mineralogy, crystallography, solid-state physics and materials science." The book consists of three parts: (1) Tensorial Aspects of Physical Properties, (2) Symmetry Aspects of Excitations, and (3) Symmetry Aspects of Structural Phase Transition, Twinning and Domain Structures. A CD-ROM containing supplementary software is also included. A list of terms and symbols as well as author and subject indices conclude the book.

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An Introduction to Chemoinformatics. By Andrew R. Leach (GlaxoSmithKline, Stevenage, U.K.) and Valerie J. Gillet (University of Sheffield, U.K.). Kluwer Academic Publishers: Dordrecht. 2003. xvi + 260 pp. $74.00. ISBN: 1-4020-1347-7.

As the authors indicate in the Preface, the term "chemoinformatics" means different things to different people. The authors' use of the term includes topics that others might associate with "molecular modeling" or "computer-assisted drug design". Thus, some readers may be surprised to see that, in addition to traditional chemoinformatic topics, this book also addresses such subjects as conformational searching, pharmacophore perception, protein−ligand docking, and even the prediction of ADME properties and toxicities. Obviously, covering such a wide range of topics within just 217 pages required numerous and very significant compromises with respect to depth.

Although the book was written for beginning graduate students and advanced undergraduates, it could certainly provide a very helpful overview for professionals with no prior knowledge of the subject matter. Almost 50% of the 444 references were published within the five years preceding publication of the book. Moreover, the authors also provide an additional list, organized by chapter, of 71 reviews, books, and articles of supplemental reading, almost 75% of which were published during that five-year period. Thus, this book could also be a useful resource even for scientists more familiar with the field.

The book is divided into nine chapters that are organized in a very logical order. Chapter 1 is a discussion of the representation and manipulation of 2D structures and includes a nice introduction to concepts related to 2D substructure searching. Chapter 2 addresses the representation and manipulation of 3D structures, including a brief discussion of methods for conformational search and pharmacophore perception. It also includes a very brief discussion of flexible 3D searching using a pharmacophore-based search query. Regrettably and ironically, the authors neglected to cover the critically important topic of stereochemistry in either of these chapters. Matters related to the chemoinformatic representation of atom-centered and bond-centered stereochemistry, the concept of local *versus* Cahn−Ingold−Prelog chirality, etc. were not discussed anywhere in the book and should certainly be addressed in the anticipated second edition.

In Chapter 3, the authors provide brief discussions of structural descriptors and comment briefly on scaling, correlation, and dimensional reduction. Chapter 4 addresses the use of structural descriptors in QSAR applications. It also includes a short explanation of partial least squares (PLS) and its application to 3D-QSAR. The last 3D-QSAR reference is to comparative molecular similarity indices analysis (CoMSIA), which leads to the topic of similarity methods that are the focus of the next chapter. In the course of discussing 3D similarity, Chapter 5 also addresses the issue of flexible 3D alignment, a prerequisite for 3D-QSAR.

The succeeding chapter begins with a reference to the often misunderstood "similar compounds display similar properties" principle introduced in the previous chapter and then presents a discussion of various methods for selecting diverse compounds for use in high-throughput screening (HTS). Chapter 7 then introduces methods for analyzing ("mining") the data generated by such HTS efforts and leads smoothly into Chapter 8, which provides a very brief discussion of methods for virtual (*in silico*) HTS. It also touches on issues of docking and scoring as well as methods for predictive ADMET. In the final chapter, the authors discuss the use of diversity methods and vHTS methods for the design of diverse and focused combinatorial libraries.

This is a rather remarkable little book. Just as its title promises, it provides (and only provides) an introduction to a very wide variety of chemoinformatic and CADD topics. It must have been quite difficult for the authors to purposefully not discuss these important topics in greater detail. The reader might occasionally feel frustrated by that lack of detail. On the other hand, that feeling of frustration would be a sure sign that the authors succeeded in whetting the reader's appetite with this clear and motivating introduction, and the authors' ample

references should enable the interested reader to satisfy his or her appetite for further details.

Robert S. Pearlman, *University of Texas at Austin*

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Annual Reports in Organic Synthesis 2003. Edited by Philip M. Weintraub (Aventis Pharmaceuticals, Bridgewater, NJ), Kenneth Turnbull (Wright State University), Jeffrey Sabol (Aventis Pharmaceuticals), and Peter Norris (Youngstown State University). Elsevier Academic Press: San Diego, CA. 2003. xxiv + 408 pp. $105.00. ISBN: 0-12-040833-3.

This handy reference presents "new, synthetically useful, or reasonably general" reactions and methods from major chemistry journals over the past year. Chapters I−III list various syntheses by reaction type, Chapter IV covers the synthesis of heterocycles, Chapter V reviews protecting groups, Chapter VI covers other synthetically useful transformations not discussed previously, and Chapters VII and VIII deal with reviews and selected "hot" topical areas. The book also includes a comprehensive table of contents, a list of journals abstracted, a glossary of abbreviations, and an index of senior authors.

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Studies in Natural Products Chemistry, Volume 29, Bioactive Natural Products (Part J). Edited by Atta-ur-Rahman (University of Karachi, Pakistan). Elsevier: Amsterdam. 2003. xiv + 902 pp. $410. ISBN: 0-444-51510-0.

This book, written by an international group of experts in various aspects of natural products chemistry, covers "synthetic approaches, structural studies as well as structure-activity relationships to a number of classes of bioactive compounds", to quote from the preface. A sampling of the topics covered includes "Ecdysteriod Structure-Activity Relationships", "Halogen-Containing Antibiotics from Streptomycetes", and "Protein and Non-Protein Protease Inhibitors from Plants". A subject index completes the book.

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