Book Reviews

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Sampling for Analytical Purposes. By Pierre Gy (Paris School of Physics and Chemistry). Wiley: West Sussex, UK. 1998. Xiv + 153 pp. $86.95. ISBN 0-471-97956-2.

The author presents an abbreviated version of his previous work entitled *Sampling of Heterogeneous and Dynamic Material Systems* (Elsevier, Amsterdam, 1992). Many mathematical proofs in the unabridged version have been omitted to create a more practical text for those working in analytical chemistry. Dr. Gy has devoted his career to this largely overlooked topic of sampling. This text highlights his theoretical and practical accomplishments as a mining engineering consultant on the subject.

The book is divided into an introduction and four parts. The introduction deals with historical perspectives of sampling and some common general sampling flaws found today, including the incorrect use of statistics and a general lack of recognition for the importance of a sampling theory. Part I provides a qualitative look at the practical aspects of reducing sampling errors that include descriptions of sample heterogeneity and homogeneity. Parts II and III take a quantitative look at obtaining reproducible samples from nonordered and ordered lots. Here the author uses his own sampling theory to quantify heterogeneity of the lot, which is necessary for determining sampling errors. Part IV deals with the author's highly recommended sampling technique of proportional sampling, which results in the obtained sample being structurally proportional to the lot. Proportional sampling was developed to overcome inadequacies found in measuring weights using belt scales and measuring volumes using dynamic volume measuring devices. Evidence is given, in terms of industrial examples, for the strong potential of proportional sampling.

The author's devotion to proper sampling is evident in this text. His descriptions and reasoning are presented logically. This book largely focuses on the sampling of moving streams of solid fragment materials; however, some theoretical correlations exist for the sampling of liquids (molecules and ions) and multiphase (fragments, molecules, and ions) mixtures. The theory presented in this book is still being tested. Further applications for sampling in other settings (i.e., environmental) will certainly strengthen the acceptance of the author's sampling theory. Dr. Gy's name will undoubtedly continue to be well recognized in the area of sampling for generations to come.

This text is strongly recommended to those who oversee or are involved in sample quality control in moving stream industrial settings. This text will also find utility for students studying sampling methods in advanced analytical chemistry courses.

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Kirk−Othmer Encyclopedia of Chemical Technology, Fourth Edition, 27-Volume Set. Wiley Interscience: New York, 1992−1998. $7884. ISBN 0-471-52704-1.

The value of the Kirk−Othmer Encyclopedia of Chemical Technology has long been so entrenched among chemists, engineers, and librarians, over the course of four editions and fifty years, that a positive review of the now-completed fourth edition almost seems automatic. Since the first edition appeared during the postwar years (1949−56), the Encyclopedia has grown and matured along with the chemical industry. The work, named for its original editors, Raymond E. Kirk and Donald F. Othmer, is a major achievement and an indispensable resource.

The first volume of the fourth edition appeared in 1992; the supplement and cumulative index volume completed the set in mid-1998. During this period, over 1500 contributors wrote new and revised articles on thousands of chemical and technical topics, some very well established, some quite new. About half the articles deal with chemical substances, either singly or as groups of compounds. The emphasis in these articles is on properties, manufacture, and uses. Other articles cover industrial processes, unit operations, chemical fundamentals, pharmaceutical and specialty products, and assorted general topics. Authors come from all sectors, but U.S. industrial R&D predominates.

The articles remain thorough and well documented, and have a consistent internal structure that makes sense to the reader in search of quick information. While most articles average 20−30 pages, some are enormous, reflecting the extensive use and development of certain classes of chemicals. (The article on inorganic fluorine compounds, for example, is 200 pages long.) The bibliographies at the end of each chapter are valuable entry points into the background (i.e. older) literature on the topic, including major patents as well as scholarly, trade, and technical publications. The currency of these references varies widely—some lists seem to stop in the mid-1980s—but Kirk−Othmer articles are not primarily intended to be literature reviews.

Cross-references at the article−title level help a browser find relevant articles, but the Index volume, which is extremely thorough and detailed, should usually be the user's first stop. Chemical nomenclature usage, as always a challenging obstacle for many publications, generally defaults to the best known correct common name for a given substance, but Chemical Abstracts Registry Numbers are universally provided within both the article text and the Index, helping reduce confusion and aiding further research. The Index lists numerous trade names as well.

Kirk−Othmer is to the disparate fields of chemical technology what the Encyclopaedia Britannica is to general knowledge. There is no more authoritative resource available. No academic or corporate entity that needs chemical information should be without this invaluable reference tool. (Libraries should make every effort, if space allows, to retain the earlier editions of Kirk−Othmer, which remain very useful as well.)

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Reviews in Computational Chemistry. Volume 12. Edited by Kenny B. Lipkowitz and Donald B. Boyd. Wiley-VCH: New York. 1998. v + 404 pp. $135.00. ISBN 0-471-24671-9.

As in the 11 volumes preceding this one, *Reviews in Computational Chemistry* proves itself an invaluable resource to the computational chemist. This series spans all the subdisciplines in the field, from techniques to practical applications, and includes reviews from many of the acknowledged leaders in the field. In this volume, as in the others, the reviews cross many subdisciplines yet are both general enough to be of wide interest to theoretical chemists while including detailed information of use to workers in particular subdisciplines.

This volume includes chapters on the following: calculations of thermodynamic properties of macromolecular systems, molecular dynamics using holonomic constraints, computational methods for water physisorption at metal−water interfaces, quantum mechanical based methods for materials simulation, quantum mechanical methods for prediction of nonlinear optical properties, sensitivity analysis in biomolecular simulation, computational methods for prediction of crystal polymorphs, and, finally, an overview of computational chemistry in France. A mixed bag of topics, perhaps, but definitely something for everyone.

The structure of this book, as in most of the volumes preceding it, is that each chapter provides first a detailed methodological approach to its topic. Rather than providing data on a particular problem *per se*, each chapter thoroughly reviews the subject matter in such a way that the reader is thereby equipped to implement the technique for his or her problem at hand, if she or he so desires. If the reader wishes only to gain general familiarity with the topic of the review, each chapter begins with an overview or introduction, which is generally comprehensive, clear, and concise. While most chapters continue on to give detailed derivations of the methods, this material is usually organized in a way that the reader may skip what is not of interest and still gain much from the chapter itself.

Of interest to this reviewer were the chapters on biomolecular simulations and water calculations. In the chapter by Meirovitch, the difficulties encountered in obtaining the thermodynamic parameters of F (free energy) and S (entropy) are discussed, as well as these

parameters' importance in interpretation of macromolecular dynamical calculations. The chapter goes on to review a comprehensive range of techniques in use for calculating these quantities, and also includes what may be reliably inferred from these data and what may not. Poring through the text, another chapter by Kutteh and Straatsma introduced this reviewer to the usage of holonomic constraints in molecular dynamic calculations. From a clear, pleasant-to-read introduction on the benefits of applying holonomic constraints to calculations on biomolecular systems, to a through overview of exactly how to implement and utilize them, this chapter inspired me to try to apply this method to some of my own calculations. Subsequent chapters were equally useful and thorough, and overall pleasant to read.

In conclusion, I believe this series has a place in every computational chemists library. This volume is no exception. Future volumes, I trust, will also continue to have the same high level of clarity and quality that computational chemists have come to expect from this series.

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Fractals in Molecular Biophysics.   By T. Gregory Dewey (University of Denver). Oxford University Press: Oxford, New York. 1997. xii + 276 pp. $65.00. ISBN 0-19-508447-0.

While it does not provide exercises or problems at the ends of chapters, *Fractals in Molecular Biophysics* is written in a nicely unified and pedagogical manner, and could certainly be used for an advanced course in this subject. It is very well-referenced, both to the literature of biophysical chemistry and to the relevant mathematical sources. The author must use a word processor that objects to long sentences, because the prose seems to this reader to be annoyingly choppy, but it is nevertheless clear. As a conventional physical chemist (not the "bio" kind), I was eager to read about what fractal analytical methods can do in the biophysical area. This book did not disappoint me. T. Gregory

Dewey makes the case, through numerous practical examples, that fractal measures and methods should be considered part of the standard repertoire of the biophysical chemist. In fact, there may not be a scientific area in which fractals will have more applications.

In the first chapter (What Are Fractals?), the author briefly reviews the mathematics of fractals. The exposition is quite condensed; a complete novice would surely want to begin by reading elsewhere. This chapter also introduces the nomenclature that is used later, reminds the reader of the phenomena to which fractals have been applied and, most importantly, emphasizes the connection between fractals and renormalization group theory. The renormalization group is used throughout the book, providing a very useful recurring theme.

Chapters Two through Four show how fractal measures provide an alternative to the traditional primary, secondary, and tertiary structure classifications of proteins, and their connection to the statistical mechanics of biomacromolecules in general. The fractal dimension seems to be a natural measure of protein structure, and one more closely related to physical measurements than are the traditional ones. In Chapter Five (Fractal Diffusion and Chemical Kinetics) the focus shifts from static to dynamical properties of biopolymers, and it remains largely in that realm through the end of the book. The fractal character of protein dynamics is described in Chapter 6, and Chapter 7 discusses fractons and vibrational relaxation in proteins. Percolation is the subject of Chapter 9 and, in Chapter Ten, Dewey explains the connection between fractals and chaos. This subject is dealt with in a brief fashion, similar to the way Chapter One is written, but the most important phenomena are mentioned and plentiful references make the treatment useful to readers looking for more depth. This volume is likely to be of interest to many readers, and should be on the bookshelf of every biophysical chemist.

Harold H. Harris, *University of Missouri-St. Louis*