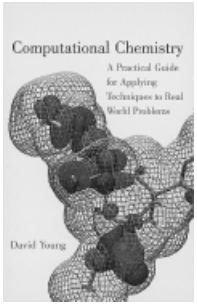
perhaps find in this book some ideas for extending their activities into new areas of application. Thus the book can certainly be recommended from that viewpoint.

Gerhard Maier
PolyMaterials AG
Kaufbeuren (Germany)

Computational Chemistry. A Practical Guide for Applying Techniques to Real World Problems. By *David Young*. Wiley-Interscience, New York 2001. 381 pp., hardcover £ 50.50.—ISBN 0-471-33368-9

Computational Chemistry—A Practical Guide for Applying Techniques to Real World Problems, by David Young, is not so much an introductory textbook but more of a concise encyclopedia in textbook form. This book covers an enormous range of methods and applications in computational chemistry. It is aimed at the experimental chemist facing real world problems that are best tackled computationally. This book is an ideal starting point for solving these problems.



The book consists of three parts: (I) Basic Topics, (II) Advanced Topics, and (III) Applications. Part I follows the general introduction (Chapter 1) and begins, in Chapter 2, with a concise outline of very basic physical concepts and theories, such as thermodynamics, quantum mechanics and the Schrödinger equation, and statistical mechanics. The chapters thereafter treat most if not all modern computational methods, ranging from molecular mechanics via semiempirical methods to ab initio methods and density functional theory (DFT). Young also discusses molecular dynamics (MD) and Monte Carlo simulations, as well as population analysis and the computation of various molecular properties (e.g., NMR parameters, boiling point, and biological activity). But also more technical issues are addressed, such as *Z*-matrix construction for geometry optimization, basis sets in ab initio and DFT calculations, and the efficient use of computer resources. Part I closes with Chapter 16, which provides some general hints on how to conduct a computational investigation.

Part II starts off with five chapters on exploring potential energy surfaces and conformations, finding transition states and computing reaction rates. Furthermore, it has chapters that deal with QM/MM approaches, solvent effects, and excited electronic states. There are also more advanced chapters on computing properties such as, for example, quantitative structure–activity relationships (QSAR), NMR chemical shifts, and nonlinear optical properties (e.g., polarizabilities and hyperpolarizabilities). As regards technical issues, Part II provides suggestions for solving SCF convergence problems, and discusses size consistency of quantum chemical methods, spin contamination, and the customization of basis sets and force fields. Finally, Part II addresses relativistic effects, band structures of crystals, mesoscale simulation of, for example, solutions or crystallization processes, as well as synthesis route prediction.

The whole is nicely rounded off in Part III with applications of the various methods to practical problems in organic, inorganic, and biological chemistry, in the simulation of liquids and polymers, and in solid-state and surface chemistry.

As already pointed out, this work is not a textbook. It simply covers too many subjects to explain them in full detail. But that is not its purpose. Instead *Computational Chemistry* serves more as a concise encyclopedia: it has an excellent subject index leading to the chapter that explains the basic features in a clear and didactic style. The reader is then referred to the appropriate scientific literature (mainly reviews and textbooks) for full details. In conclusion, Young has written a very useful guide that assists advanced undergraduate and graduate students, but certainly also professional (experimental) chemists in conducting computational research projects in almost all areas of chemistry.

F. Matthias Bickelhaupt
Scheikundig Laboratorium
Vrije Universiteit
Amsterdam (The Netherlands)

Biotechnology. Vol. 5b. Genomics and Bioinformatics. Edited by *Christoph W. Sensen*. Wiley-VCH, Weinheim 2001. xvi + 462 pp., hardcover € 279.00.—ISBN 3-527-28328-5

When a book goes into a new edition after only a few years, it is an indication that it deals with a highly topical and rapidly developing area of work. However, in this case all comparisons fail to do justice to the situation. The combined subject index to the first edition of the eight-volume work *Biotechnology*, published in the period 1981–1989, did not contain the words genomics, proteomics, or bioinformatics! Now the new edition of the work, started in 1993, is complete. At the beginning of 2001, coinciding punctually with the announcement in *Nature* and *Science* of the determination of the human genome sequence, Volume 5b (*Genomics and Bioinformatics*) appeared, along with the index volume for the whole work.

The determination of the human genome sequence is only the first step in genome research. We read the letters, and we understand their meaning in many cases, but we do not understand the language itself. That is rightly emphasized repeatedly in this volume. The chapters, all written by top-class authors, deal expertly and concisely with every aspect of genome research, including especially their medical implications, and with proteome research and bioinformatics.

The section on applications contains a chapter reviewing the genome project for various model organisms (*E. coli, B. subtilis, Archaeoglobus fulgidus, S. cerevisiae, A. thaliana, C. elegans*, and *Drosophila melanogaster*), a chapter on the human genome project, two chapters on monogenic hereditary diseases and the predisposition towards certain diseases due to polygenic changes in the genetic make-up, a chapter on pharmaceutical bioinformatics and the discovery of new active agents (although this is mainly concerned with target identification and analysis rather than with searching for new active agents), and lastly a chapter on genome research in agriculture, an aspect that generally receives too little attention. The section on DNA technologies contains chapters on gene

  1433-7851/02/4102-0365 $ 17.50+.50/0

mapping and positional cloning, with the main emphasis on plant genetic engineering, on sequencing methods, and on DNA microarray techniques in research. Next comes a section on protein technologies consisting of two chapters on important techniques, namely two-dimensional gel electrophoresis and mass spectrometry for proteomics and proteome analysis using capillary electrophoresis. This is followed by a section on bioinformatics, containing first a review of the use of molecular biological data, then two chapters on bioinformatics tools for genomics and proteomics, and a chapter on structural information, dealing with the recognition of function, determination of folding pattern from the sequence (threading methods), homology modeling, and virtual screening. This section also includes specialized chapters on automated gene annotation and complete genome comparison, graphical representation of genome data (e.g., using MAGPIE), and data banks on protein–protein interactions. The book ends with a section on the ethical, legal, and social aspects of genome research, consisting of a chapter on ethical aspects and commercial genome data banks, and a chapter entitled "Genomics—Five Years from Now", which considers the outlook for future developments in this field.

The book is not in itself especially suitable for beginners in the subject. Some important fundamentals (e.g., the polymerase chain reaction) are not described in detail. To learn about these the newcomer also needs to refer to other books in the series or to a more recent textbook. However, for readers who already have a basic knowledge of biochemistry and molecular biology, and especially for those already working in this field, the book offers a wealth of information in a concise form. As one expects in a multiauthor work, the contents of the chapters overlap in a few areas, whereas other topics (e.g., gene shuffling and error-prone PCR as methods for altering genetic properties for specific purposes) are not covered. Nevertheless, that certainly does not diminish the overall merit of the book. The errors are very few and are no more than spelling mistakes or typos (e.g., p. 172, Fig. 1: "Phisycal Map"). The book is remarkably up-to-date, as the literature coverage extends into 2001. The format of the literature citations is very useful, as it includes titles of papers and articles. All the chapters refer the reader to appropriate review articles published within the last two years.

This book can be recommended unreservedly to everyone who wishes to gain an overview of the current situation in genome and proteome research, including the methods of bioinformatics. It will be very useful to chemists, biochemists, molecular biologists, medical researchers, and scientists involved in research in the pharmaceutical and agricultural fields.

Hugo Kubinyi
Weisenheim am Sand (Germany)

Colour Chemistry. By *R. M. Christie*. Royal Society of Chemistry, Cambridge 2001. xii + 206 pp., softcover £ 19.95.—ISBN 0-85404-573-0

Color chemistry is an area of research and technology that can now be described as mature. Evidence for that includes not only the restructuring of the industry and the shift of manufacturing to Asia, but also a steady decline in the rate of publications in this field. The most recent major monographs on the subject are already about ten years old. So have there been so many recent developments that the publication of a new comprehensive overview is worthwhile?

In this book of about 200 pages R. M. Christie has aimed to give a clear and didactic survey of dyes and pigments, which is intended for students and for chemists who wish to become involved in the area. After an introduction to the history of the subject and to the physicochemical fundamentals of color chemistry, the author describes the most important chemical structures present in dyes and pigments and methods for synthesizing them. Some relatively new chromophores that were introduced in the 1980s or later are also described.

That is followed by three chapters describing the most important physicochemical processes involved in using dyes and pigments, with particular emphasis on textile dyeing and the processing of pigments. The application of colors to paper and leather is also treated, but more briefly. It is regrettable that the author includes scarcely any discussion of thermodynamic and kinetic aspects of the dyeing process, presumably for reasons of space.

However, "functional dyes" used in advanced technological applications are discussed in more detail. These attract special interest against the background of the maturity and relative lack of innovation in other areas of color chemistry. Although not all the examples described here represent the very latest state of the art, they are presented skillfully and instructively, with clear and detailed explanations, and they serve to illustrate the wide range of possibilities.

The final chapter deals with environmental and toxicological aspects. Effluent disposal problems in the production and use of dyes are discussed briefly and in a very condensed form. Methods for removing dyes from wastewater are described or proposed. This chapter also is too brief—for example, it should include a list of aromatic amines that have been incriminated.

Considered as a whole, this survey touches on nearly all aspects of modern color chemistry. However, lack of space has meant that many aspects are treated only qualitatively, and consequently in a rather superficial way. Also the absence of color illustrations does not make for easy readability. A good aspect of the book is that the author suggests likely mechanisms for many industrially important dyestuffs syntheses. The usefulness of the book could be greatly improved by providing references to recent papers and review articles, and it could then serve as a good introduction to working in the field of color chemistry. The list of textbooks at the end, without corresponding references in the text, is not enough. This work by Christie is more a textbook than a monograph, and therefore it is mainly suitable for students interested in color chemistry.

Günther Seybold
BASF AG
Ludwigshafen (Germany)

  1433-7851/02/4102-0366 $ 17.50+.50/0