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.

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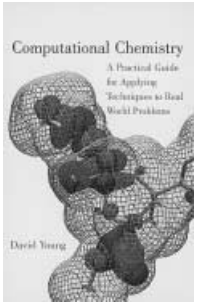
Computational Chemistry. A Practical Guide for Applying Techniques to Real World Problems. By *David Young*. Wiley-Interscience, New York 2001. 381 pp., hardcover £ 50.50.—ISBN 0-471-33368-9

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.

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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

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