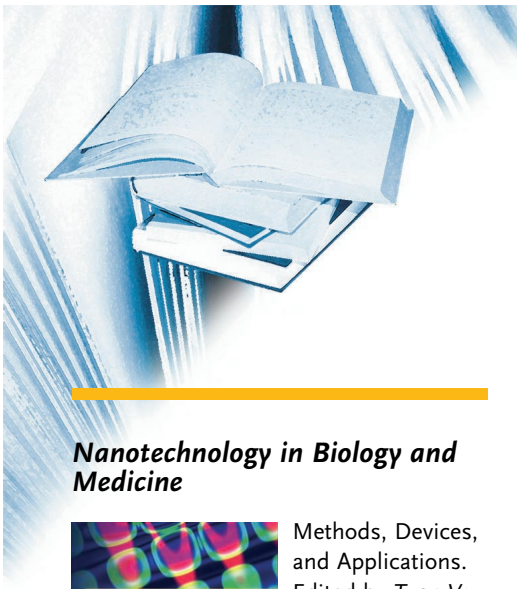
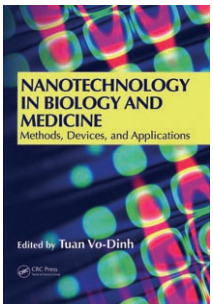


Nanotechnology in Biology and Medicine



Methods, Devices, and Applications. Edited by *Tuan Vo-Dinh*. CRC Press/Taylor & Francis, Boca Raton 2007. 616 pp., hardcover $ 149.95.—ISBN 978-0-8493-2949-4

During the last decade the emerging field of nanotechnology has started to influence and revolutionize many areas of science. Nanotechnology concepts are particularly interesting for the life sciences, where the fact that artificial nanostructures and biological structures often have similar dimensions allows an efficient intercommunication between nanotechnology, biology, and medicine.

This timely book is a collection of 39 chapters dealing with different aspects of nanotechnology in biology and medicine. The contributions are arranged in two sections. Section I is entitled "Nanomaterials, Nanostructures, and Nanotools", while Section II deals with "Applications in Biology and Medicine".

After an introductory chapter written by the editor, the first chapters discuss various nanostructures with an emphasis on their biomedical applications. These include: self-assembled organic nanotubes; silicon, gold, and bimetallic nanoparticles; nanowires; quantum dots; and various more complex bio-inspired nanomaterials and nanodevices, such as nucleoprotein-based nanodevices for drug delivery, and nanotube-based membrane systems.

A second group of chapters in Section I focuses on new nanotechnology-based tools and methods, such as nanopore methods for DNA detection and sequencing, and describes processes for the manipulation and deposition of single biomolecules. One chapter is devoted to biological applications of scanning transmission electron microscopy (STEM).

Powerful tools for biomedical research can be built by combining nanotechnology and optics. Several chapters in the book address this bio-nanophotonics aspect by discussing optical nanosensors and nanoprobes, and observations of single molecules in cells by optical spectroscopy. Particular emphasis is given to plasmonics-based approaches, in chapters on topics that range from sensing of biomolecules by surface plasmon resonances to nanoscale imaging of biomolecules using near-field scanning optical microscopy, and to cellular imaging and gene detection using surface-enhanced Raman spectroscopy (SERS), a method described in Section II of the book. This second section is intended to focus more on applications. Some more general chapters in Section II are entitled "Nanoparticles in Medical Diagnostics and Therapeutics", "Nanotechnologies in Adult Stem Cell Research", and "Integrated Cantilever Based Biosensors for the Detection of Chemical and Biological Entities". Other chapters in Section II cover topics such as bioconjugation of nanoparticles, techniques for monitoring apoptosis and anticancer drug activity, the use of quantum dots as tracers for DNA electrochemical sensing systems, and the role of carbon nanotubes in bio-electrochemistry.

Individual chapters in the book are between 10 and 25 pages in length. In most cases, they are easily accessible and can be read as individual articles independently from each other. The arrangement of the chapters in two sections appears to be somewhat arbitrary, and sometimes the reader may even find it confusing. Section I of the book contains some interesting applications, while Section II also includes introductory chapters on nanomaterials, nanostructures, and nanotools. For example, nanoshells and carbon nanotubes are introduced in Section II.

Overall, this book with contributions by 96 authors from a broad range of disciplines is a valuable resource for everyone interested in this exciting interdisciplinary field, where nanotechnology and optics meet biology and medicine. As it gives detailed information about various sensing methods and analytical techniques, as well as extensive references, it will be useful for researchers and students who want to get started with their own projects based on nanotechnology approaches for addressing biological and medical questions.

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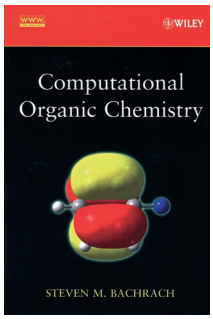
Computational Organic Chemistry



By *Steven M. Bachrach*. John Wiley & Sons, Hoboken 2007. 478 pp., hardcover € 97.90.—ISBN 978-0-471-71342-5

For any book on computational chemistry, or more generally on theoretical chemistry, it has to be decided at the outset whether it is to concentrate in detail on the fundamentals or on the applications. This dilemma arises because an attempt to cover both parts in detail inevitably results in a very thick book, which is often undesirable from the viewpoints of both the publisher and the author. In his book, Professor Bachrach has settled firmly on the side of applications. However, since the book also concentrates on certain topics where newer methods of calculation have revealed new aspects, there is also an additional focus, of a kind that one might not expect from the general-

sounding title Computational Organic Chemistry. That fact already leads to a short verdict: if one expects the book to provide a comprehensive description of "computational organic chemistry", then one will be disappointed. If, on the other hand, one expects to find carefully selected case-study examples whereby the capabilities and limitations of different theoretical approaches are described in detail, then one will be very satisfied. For conveying an understanding of the underlying theory, or as a detailed presentation of all aspects of theoretical organic chemistry, this book is only of limited use. On the other hand, it is the right book for the reader who wishes to get a feel for deciding which of the standard theoretical approaches that are available in existing program suites is best for a given organic chemistry problem.

As examples of the book's coverage of organic chemistry as a whole, there are chapters on pericyclic reactions (Chapter 3), diradicals and carbenes (Chapter 4), organic reactions of anions in the gas phase (Chapter 5), and the effects of solvents on the structure and reactivity of organic molecules (Chapter 6). In addition there are discussions about some selected fundamental concepts of organic chemistry (Chapter 2), and a chapter on reaction dynamics (Chapter 7). Preceding all this is an introduction to the theoretical methods of computational organic chemistry (Chapter 1). It is already apparent from this list of chapters that the author has not tried to give a comprehensive description of computational organic chemistry, but has concentrated on some chosen case studies as examples. This becomes clearer if we consider Chapter 3, "Pericyclic Reactions". From this general title one would perhaps expect a description of the fundamental theoretical studies by Hoffmann, Fukui, Zimmermann, and Dewar, or perhaps instead a broad-ranging treatment of the different individual reaction types. The chapter is neither of these. Instead this book concentrates on calculations for just a few reactions which, according to the author, either have provided new insights or allow a very reliable evaluation of the accuracy of the theoretical methods used. Chapter 3 continues with about 13 pages on torquoselectivity, and 17 pages on the Bergman cyclization and related reactions. However, there is not a single line on (for example) sigmatropic shifts of hydrogen atoms. Although the choice of subject matter may have an inner consistency, it does not necessarily reflect the relative importance of the individual topics, and therefore probably not the expectations of potential readers.

The strength of the book lies in the very detailed discussion of the case examples, the comparison of different methods with regard to the results that they can give, and in many cases also an explanation of the reasons. The author's approach is well illustrated by two examples of reactions, the Diels–Alder reaction and the Cope rearrangement (Chapter 3). Table 3.1 contains 51 different calculations of the activation energy for the concerted reaction of 1,3-butadiene and ethene. As the theoretical methods range from simple Hartree–Fock calculations to MR–AQCC approaches, the table enables one to arrive at precise conclusions about which methods are suitable and which are not. Similar discussions exist about the various reaction pathways of the Diels–Alder reaction, the effects of substituents, and the question of when the reaction proceeds synchronously and when asynchronously. The treatment of the Diels–Alder reaction is rounded off very nicely by the discussion about solvent effects, which one finds in Chapter 6. The discussion of the merits of the different methods of calculation extends to the question of how the calculated reaction profiles can be influenced by a superposition error in the basis set, a question that is seldom considered. There is a discussion about the trends that are observed, which helps the reader to some extent in carrying the knowledge over to apply it to other cases. But only to some extent, because the author of this book, like other authors, fails to explain why DFT, in particular the hybrid-functional variant B3LYP, yields such good results (see also the discussion about the Cope rearrangement). However, to his credit it must be added that at this point he warns the reader not to use the Cope rearrangement as the single benchmark example.

Chapter 1, which is intended to introduce the reader to theoretical methods, is not very effective. It is too superficial, and is more an exercise in namedropping than a proper discussion of the methods. The author himself admits this, and recommends that one should study other books. However, I find this chapter unsatisfactory for other reasons, as two examples will show. The variational principle is not introduced until after the Hartree–Fock method, which is confusing because the Hartree–Fock method itself is an important application of the variational principle. More consistently, the Hartree–Fock method is also introduced as an application of an effective operator, rather than simply as a method for minimizing the energy as a function of the orbitals if one uses only one Slater determinant. Another faux pas occurs with the density function theory, where the author refers to the density without having previously defined it.

As a way of sketching the "human interest" behind the science, the book contains six subchapters in which the author presents interviews with researchers who have contributed significantly to the topics of the individual chapters. These interesting additions round off the book nicely.

A book review must always address the question of which readers will benefit from the book. Professor Bachrach states that he has written it for a very wide readership, from experts to final-year or graduate students. In particular, he writes that the reader does not need to be an expert to benefit from the book. With regard to the breadth of the readership, I am rather skeptical. The book contains so much detail that an experimental chemist who does not have much previous experience with calculations (and their theoretical background) will be simply overwhelmed. Since the amount of detail included has prevented detailed discussions of all the trends and sources of error, those readers who are already familiar with the acronyms (although not yet with their theoretical background) will still have difficulty in understanding the potential error sources sufficiently to avoid falling into similar traps in their own calculations. On the other hand, if one's knowledge of both (acronyms and the background) is fairly sound, then the book offers a real gain. Leaving aside the above reservations about the choice of topics, every research group that wishes to carry out its own calculations should have access to this book, as it is one of the few books that describes in detail which methods can yield which kinds of results. However, at the same time one must work through the standard books on the fundamentals of theoretical chemistry, as a good knowledge of theoretical methods is necessary in order to use this book effectively.

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