Computational Organic Chemistry; by S. M. Bachrach, John Wiley & Sons: Chichester, **2007**, hardcover, 496 pp, € 92.90, ISBN 978-0-471-71342-5

Steven Bachrach's book is not another introduction to computational methods but rather a collection of cases in which these have been fruitfully applied to organic reactivity. In the light of a still-growing number of published computational studies of organic reactions, this new kind of presentation delivers a compilation of examples of what can successfully be achieved with quantum chemistry. Semiempirical and force field methods are left out.

In the first chapter, the reader finds a "brief and mathematically light-handed treatment" of the underlying theory. Most standard methods and concepts are introduced on 37 pages [Hartree–Fock (HF), post-HF methods, composite theories, DFT, basis sets and BSSE, electronic properties]. Of course, this presentation is not comprehensive and has to omit some facts. For instance, the formula of the MP2 correlation energy, which would be very instructive to understand the advantages and pitfalls of that widely used method, is absent. The author himself explains that the introduction is meant to deliver a general understanding to those unfamiliar with quantum chemical methods. He recommends certain other textbooks for more depth and details. Indeed, to get a concise understanding of how the methods work, the reader will have to consult another introductory book about quantum chemistry.

The remainder of Bachrach's textbook deals with the application of computational methods to selected topics of organic chemistry. The second chapter introduces fundamental concepts of organic chemistry such as bond dissociation energies, ring strain and aromaticity. As in all following chapters, for many calculated quantities results with different methods and basis sets are discussed, giving the reader an impression of the quality of particular approaches. The presentation is unbiased and does not conceal problems and failures of widely used methods: quite early, on the fourth page of chapter two, the reader is confronted with the failure of the popular B3LYP functional to predict alkane bond dissociation energies. In that sense, the presentation will be enlightening for some readers who have too much confidence in specific 'black box' approaches. What one misses is more specific information about the computational cost of the calculated quantities. Readers choosing a method for their studies would like to know 'at what price' the numbers can be obtained.

In the following parts, classical topics of organic reactivity are discussed from the computational perspective: pericyclic reactions (chapter 3), carbenes and radicals (chapter 4), anions (chapter 5), solvent effects (chapter 6) and reaction dynamics (chapter 7), each chapter consisting of a number of specific case studies.

Chapter 3 presents studies of the Diels–Alder, Cope and Bergman reactions, as well as electrocyclic reactions. The examples of anion chemistry (chapter 5) include studies of stereoselectivity in nucleophilic additions and catalyzed aldol reactions, illustrating that the right transition state model is crucial for understanding selectivities. Computational methods are highly relevant tools for revealing reaction mechanisms and reasons for observed selectivities.

The two final chapters include short presentations of the theoretical models that are employed: implicit solvent models (chapter 6) are introduced and aqueous Diels–Alder reactions are discussed. Conformational equilibria and tautomerism of biomolecules (glucose, nucleic acids) are nicely chosen examples where solvent effects play a decisive role. The final chapter (7), about the computation of molecular dynamics, contains a short methodological introduction and quite a few well-chosen examples of non-statistical product distribution. It nicely represents a compact and comprehensible overview of this important topic.

In all chapters, large numbers of references are given for both theoretical basics and the presented cases, amounting to over 100–150 at the end of each chapter. In that way, the reader obtains an extensive list of starting points for further literature studies. The list is also available on a web site with links to journal references. On the same site, a blog with more recent literature examples offers a platform for further study and dialogue with the author.

One could easily set up a list of topics that are not discussed in the book – such as radical stabilities, rearrangements of carbocations and reactions of transition-metal compounds. Maybe some will find their way into a later edition. However, the goal of this book is to introduce the reader to the application of computational methods and this is well achieved without presenting an encyclopedic compilation of applications.

An excellent idea was to conclude each chapter with an interview of a researcher who has contributed to the field of computational chemisty, leading the reader behind the stage of science. Such 'human' aspects are usually not contained in textbooks. The reader looks into the development of computational chemistry and sees how it has been conceived by the persons involved.

Computational Organic Chemistry is highly recommendable, I have enjoyed reading the book from the first to the last page. Organic chemists and graduate students planning the use of theoretical methods in combination with experimental research will benefit a lot from studying it thoroughly. It will also help theoretical chemists remember that their methods always have to survive the comparison with 'real life' (large molecules, solvent effects, etc.).

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