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Book Review

STEVEN M. BACHRACH

Computational Organic Chemistry

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A well written, interesting book which takes a case study approach to demonstrating the power and importance of computation in organic chemistry.

The book is largely aimed at an audience with a background in organic/physical organic chemistry, rather than those coming from a more theoretical base. As such it is written as a series of case studies, which highlight how computational chemistry can support experimental organic chemistry as well as providing new insights into mechanism and reaction prediction.

The book begins with a brief introduction to each method discussed within the case studies, but glosses over much of the mathematics that underpins the subject. Bachrach explicitly states that this is to provide those who are not already familiar with the area with a general understanding of the methods, concepts and acronyms that are so widely used. On the whole he is successful in his aim. By simplifying the discussion, the physical interpretations of the strategies become clearer. This enables the reader to understand the methods in a way that makes appreciating their relative merits and suitability for a given problem much easier. One notable absence however, is that of a summary or glossary of this section for easy reference by the reader when reading the rest of the book.

Some of the more fundamental problems in organic chemistry (acidity, ring strain energy, aromaticity) are discussed with appropriate examples, before the book moves on to its main purpose: case studies.

Major reaction classes are discussed in turn, including, pericyclic, radical and ionic. In each case, the reader is taken through well chosen and well referenced examples in an easily accessible, narrative form. The focus is largely on the choice of method, reinforcing an underlying theme of the book: to educate the reader on selection of appropriate strategies for a particular problem. The narrative approach makes the book an entertaining read and easily accessible to those who have little experience of computational chemistry. The discussion of the development of the various models for asymmetric addition to carbonyls is particularly interesting and well presented.

The scope of the book is limited to *ab initio* and DFT methods only. This partly a practical consideration and partly a look to the future with molecular mechanics and semi-empirical methods starting to take a back seat in computing systems of interest to organic chemists. Reference is made in several places to the importance of covering all configurational space, notably in the chapter devoted to solution-phase chemistry, but there is virtually no discussion of the methods available to do this. Case studies deal with simple systems, as is usual within computational organic chemistry but a discussion of the need to simplify the systems which are to be studied and what are/are not appropriate simplifications is missing. In a similar vein there is little discussion of the comparative computational cost of the different methods discussed throughout the book, which is surprising given the otherwise excellent coverage given to comparing the suitability of the different approaches.

Each chapter on a particular topic is book-ended by an interview with a leading figure in current computational organic chemistry, often one who has been a major player in the field(s) discussed. This makes an interesting counterpoint to the narrative structure of each chapter, and lets the individual characters of those involved in pushing forward the field come through. Two small criticisms of this approach might be i) the researchers chosen for interview are solely from the USA; and ii) the match of researcher to chapter sometimes seems slightly artificial.

This is not a reference text. Rather, it is a very well written and enjoyable journey through some of the successes of computational organic chemistry. It gives an overview of what can be achieved leaving the reader in no doubt that computation is an important tool for both the synthetic and physical organic chemist.

John Brazier James Platts
Cardiff University, UK