Book Review

1 PERKIN

Essentials of Computational Chemistry. Theories and Models

Christopher J. Cramer, Wiley, 2002, xvii + 542 pp.,
price $45 (paperback), $110 (hardcover), ISBN 0-4714-8552-7

Several books have appeared in recent years that give an overview of different methods used in computational chemistry, rather than giving an in-depth treatment of a specific subfield of theoretical chemistry. *Essentials of Computational Chemistry* by Christopher Cramer is a recent addition to this trend, and provides an excellent example of how the mainstream computational chemistry models can be introduced to the novice.

The book contains 542 pages and is divided into 15 chapters and 4 appendices. Each chapter has a short 1–2 page introduction to the topic, a more detailed review of the theory behind the model, and finishes with a 2–3 page case study of how the model can be used for a specific problem. Personally I find this an excellent approach for introducing new and often difficult theoretical concepts. Many chapters include a discussion of the strengths and weaknesses of the methods, as well as examples drawn from the literature. In addition each chapter contains a short list of books and reviews, which can be consulted for more details, and a slightly longer list of specific references to articles in scientific journals. The style and language make reading easy, and no extensive mathematical background is required to follow the flow of the arguments. Equations are used relatively sparsely, concentrating on the essential formulae, and few actual derivations of equations are provided. Reference is made to recent papers describing on-going developments and calibrations, making it easy for the reader to seek further information. The chapters are furthermore relatively self-contained, making it possible to read only the topics of interest, and allowing the book to be used as a required or supplementary textbook for a course. It also appears to have been carefully proof-read, at least I have failed to spot any obvious errors.

The book clearly focuses on application of computational models to solve chemical problems, and is not a reference text for theory developments. Although the author introduces most of the quantum mechanical and mathematical tools used, I recommend that the reader has some prior knowledge of elementary quantum mechanics, calculus and linear algebra to realize the full potential of the book. The book does not focus on any specific software packages, although references are made to specific computational models and programs. There is very little in terms of guidelines for how to estimate the computational resources required for a specific problem, although the case histories give some illustration of the capabilities of modern technology.

There are two main topics in the book, quantum electronic structure theory and treatment of condensed phases, the latter being equated with liquids and solutions in the present case. These two topics occupy 10 of the 15 regular chapters, with the remaining 5 dealing with an introduction, molecular mechanics, spectroscopic properties, hybrid QM/MM methods and models for calculating rate constants. The 6 chapters describing different approaches for solving the electronic Schrödinger equation have the main focus on independent particle models (Hartree–Fock, Density Funtional Theory, semi-empirical methods), and less on advanced theoretical models for treating electron correlation. A chapter on thermodynamics provides the basic theory for understanding the connection between the microscopic and macroscopic worlds, and 3 additional chapters discuss details of simulations and implicit and explicit models for condensed phases. Finally the 4 appendices contains a list of acronyms in computational chemistry, a section on symmetry and point groups, spin algebra and orbital localization.

The main focus of the book is on the use of theoretical models to calculate molecular structures and energetics, which is by far the most common use of computational chemistry methods by non-specialists. The selection of methods included also favors those which intuitively are the easiest to understand, *e.g.* independent particle models like Hartree–Fock and Density Funtional Theory, rather than advanced methods like coupled cluster. The latter occupies only 3 pages in the book, despite being one of the currently most successful methods for achieving highly accurate results. More specialized topics like electric and magnetic properties, relativistic effects, periodic systems and structure–activity relations are touched only briefly or not at all. Furthermore, the main part of the examples included is organic by nature and of small and medium size, *i.e.* not proteins and DNA/RNA.

As always the selection of topics included in a book depends on the author's own interests, but in the present case the choice very nicely reflects the mainstream of modern computational chemistry as used routinely in many areas of chemical research. With a price of $45 USD for the paperback version, this is a book which should find its way to the bookshelf of all researchers who use computational chemistry tools, as well as being an excellent choice as a textbook for a upper undergraduate or graduate course in computational chemistry.

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