Book & Media Reviews

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Molecular Modeling on the PC

by Matthew F. Schlecht

Wiley-VCH: New York, 1998. xviii + 763 pp. ISBN 0-471-18567-1. $79.95

reviewed by Frank Rioux

"Computer-aided molecular modeling doesn't exist for its own sake, but to contribute to scientific endeavor, and enable the scientist to work smarter." This is the last sentence of Schlecht's preface and it says something very important about contemporary scientific research in the academic and industrial venues. Owing to the accelerating improvement in computer technology (hardware and software) and its widespread availability, molecular modeling has become a reliable and important tool in chemical research. Consequently, experimentalists have incorporated molecular modeling techniques in their research, and partnerships with computational chemists have become common.

This is a well-organized and thorough monograph that devotes its attention to one type of molecular modeling, molecular mechanics, and one molecular modeling software package, PCMODEL. Schlecht targets two reader–user groups, the novice and the journeyman modeler, and articulates three goals. He wants to provide the novice with an introduction to molecular mechanics, and after that with some practical examples of the use of empirical force field calculations. His third goal is to provide the journeyman modeler with a reference work that will aid "further study and practice".

These are potentially conflicting goals, but Schlecht is, in my opinion, successful because of the way his book is organized. A comprehensive treatment such as this one is not meant to be read from cover to cover, because it is both an exposition of basic principles and a user's manual. Therefore, the novice and the experienced modeler will undoubtedly use this book in different ways. For example, a novice modeler might be advised to read the Preface and Chapter 1, which together provide a broad introduction to the historical development and goals of molecular mechanics. From there the novice could go to Chapter 5 and read section 5.1 on the components of the molecular mechanics force field, which is presented in 22 pages with plenty of graphical support. The reader is now ready to move to Chapter 6 on applications and work through the 32 exercises (Chapters 3 and 4 have an additional 11 exercises) designed to illustrate the current uses of molecular modeling in academic and industrial research. Chapter 3 (Input and Output), Chapter 4 (File Formats), and the balance of Chapter 5 can be consulted as needed. For example, Chapter 5 contains 160 pages on the evolution of the various empirical force fields in use today and important information in each case on parameterization and implementation.

Besides finding a clearly written, well-organized, thorough presentation, the reader will appreciate a number of other important features. There are numerous references (993) to the primary literature covering the field of molecular mechanics from its beginnings to mid-1997, when the book went to press. There is a complete glossary of PCMODEL commands, and a comprehensive and valuable glossary (77 pages) of frequently used computer terms. There are 392 figures (many of them screen captures) providing illustrations of the PCMODEL interface in use and examples of input and output files. To aid the reader/user in obtaining expertise as a modeler, a diskette containing all the structure files for all the exercises accompanies the text. In addition, the author provides, on the same diskette, a browser-readable HTML file that contains links to a large number of pertinent resources on the World Wide Web.

In summary, *Molecular Modeling on the PC*, by Matthew Schlecht, is a very impressive contribution to the molecular modeling literature. Schlecht's book should be in every college and university library and in the personal libraries of those who want to learn more about molecular mechanics or who anticipate its use in their teaching or research.

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