Book Reviews

Computational Chemistry Using the PC. Third Edition. By Donald W. Rogers. John Wiley & Sons, Hoboken, NJ. 2003. xvii + 349 pp. 16 × 23.5 cm. ISBN 1-471-42800-0. $69.95.

In the preface to this, the third edition of Donald Rogers' popular text on exploring computational chemistry on a PC computer, the author states: "One does not have to work at one of the world's select universities or research institutes to do world class research. Your research equipment now consists of an off-the-shelf microcomputer and your imagination." It is in this spirit that this book sets out to make accessible the field of computational chemistry. All that is needed is simply an inexpensive PC, Internet access, and an abiding interest. Professor Rogers' treatment of the material is excellent, and this complex subject is presented in a clear and concise manner. This text is highly recommended for those interested in teaching courses in computational chemistry.

This is the third edition of a textbook that was first published in 1990, and to the credit of the author, this edition stays, for the most part, current with developments in a relatively rapidly changing field. The book is targeted to an introductory audience, and it is well suited to be used in conjunction with courses for senior-level undergraduate students or possibly as an initial or remedial text for a graduate-level program. The introductory chapters consist of a review of those areas of mathematics that are important for students to comprehend if they are to grasp the computational chemistry concepts that are introduced later. Included in each chapter are both computer projects and exercises illustrating both the mathematical and the chemical concepts.

The focus of the book is primarily on how computation can be brought to bear on the problems of modeling relatively small molecules, including coverage of molecular mechanics, molecular orbital theory, a strong treatment of molecular orbital calculations, and quantum chemistry. The subjects are introduced at a relatively sophisticated level, and a high level of chemical understanding is assumed, which is appropriate given the intended audience. There are a few small problems with this book, which may cause some frustration for instructors who may wish to use it as primary course material. The BASIC programming language was an appropriate choice for an introductory language a few years ago, but with the proliferation of open source software, an instructor designing a course from scratch might choose to base the material on a more advanced language such as Python or Perl.

Nonetheless, this text is a real gem, and it should be considered by anyone contemplating developing course materials in the area of computational chemistry.

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