Book Reviews

Reviews in Computational Chemistry. Volume 1 and Volume 2. Edited by K. B. Lipkowitz and D. B. Boyd. VCH Publishers, New York. Volume 1: 1990. xix + 419 pp. 16 × 24 cm. ISBN 0-89573-754-X. $125.00. Volume 2: 1991. xvi + 527 pp. 16 × 24 cm. ISBN 1-56081-515-9. $105.00.

Computational chemistry is a relatively new multidisciplinary area of research that offers a variety of tools and techniques that are becoming increasingly more important to medicinal chemistry. The numbers of publications, workshops, and symposia concerning aspects of computational chemistry are continually growing and provides the incentive for a published resource to keep track of progress in this area.

The goal of the editors of these two volumes is 2-fold. The first is to provide a mechanism where someone unfamiliar with computational chemistry can be brought quickly up-to-date. The second is to provide a reference for experts wishing to keep abreast of new developments. It should be emphasized that both volumes are geared toward the organic and pharmaceutical communities. The articles contained in both volumes consist primarily of tutorial-like introductions rather than exhaustive reviews of the current literature. Areas that are covered in the first volume include ab initio methods, semiempirical quantum chemistry, QSAR, chemometrics, chemical databases, and molecular surfaces. The second volume contains articles on conformational analysis, molecular mechanics, molecular dynamics, quantum chemistry, and QSAR. Both volumes provide an appendix containing information on available molecular modeling software organized by the types of computer required.

In volume 1, chapter 1 by Feller and Davidson describes basic principles for selecting basis sets for ab initio Hartree–Fock calculations. Chapter 2, by Stewart, discusses semiempirical methods proposed by Dewar. In chapter 3, Dykstra et al. examines the calculation of molecular properties by direct calculation. In the fourth chapter, Plummer describes the use of theoretical aids such as statistical methods to the design and synthesis of new pesticides. Jurs, in chapter 5, provides a comprehensive overview of chemometrics. In chapter 6, Martin et al. describes the construction and use of 3D chemical databases. Mezey, in chapter 7, describes theoretical models for characterizing molecular surfaces. Chapter 8, by Lybrand, discusses molecular simulation methods involving perturbation theory and molecular dynamics in the calculation of free energies. The ninth chapter, by Boyd, describes various aspects of molecular modeling. Boyd, in chapter 10, describes the usefulness of computational chemistry and in particular describes the development of four compounds which depended quite heavily on computational methods. In the final chapter, Davidson discusses perspectives on ab initio calculations and attempts to answser the question of what can be learned and what has been learned through 35 years of quantum chemistry. An appendix, as noted above, lists software available to support molecular modeling on various computing platforms.

In volume 2, Leach, in chapter 1, provides a review of methods for searching the conformational space of small to medium-sized molecules. In the second chapter, Troyer and Cohen survey several methods for predicting the structure of proteins and describe several of the problems associated with such predictions. Chapter 3, by Bowen and Allinger, describes the theory, history, and formulation of molecular mechanics in the development of the MMI, MM2, and MM3 force fields. These force fields are especially applicable to the study of small organic molecules. In chapter 4, Dinur and Hagler describe the progress in developing improved force fields applicable to macromolecules. Scheiner, in chapter 5, describes molecular mechanics methods for calculating the properties of hydrogen bonds. In chapter 6, Williams describes the use of net atomic charge and multipole models to estimate the ab initio molecular electric potential, which is critical in the study of intermolecular interactions. Politzer and Murray, in chapter 7, review molecular electrostatic potentials and chemical/biological reactivity. In chapter 8, Zerner describes many of the semiempirical molecular orbital methods in use today. Hall and Kier, in chapter 9, describe the use of molecular topology descriptors (χ connectivity indices and κ shape indices) in structure–property modeling. Bersuker and Dimoglo review in chapter 10 the so-called electron topological method of prediction of biological activity. Chapter 11, by Boyd, reviews some of the key papers in computational chemistry and attempts to ascertain important trends among the journals that focus on this field. As in Volume 1, an appendix is included that contains an updated list of molecular modeling software organized by the type of computing platform required.

The standard of production for both books is excellent. There are many references to key publications in all chapters. In addition, both books contain an author index and a subject index. Many diverse areas of computational chemistry are covered in the two volumes, but some emerging techniques, such as the development and application of molecular similarity analysis, are so far unrepresented. In summary, the editors are to be congratulated for collecting the several excellent review articles on topics of current interest that are contained in these two volumes. Both books are highly recommended to the practicing chemist who have little or no knowledge of the tremendous impact that computers have made in medicinal chemistry.

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