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Book reviews

K. B. Lipkowitz, D. B. Boyd (eds) Reviews in Computational Chemistry. Vol. 1. VCH, Weinheim, 1990, 419 pages, 66 figures, 59 tables. DM 176

The aim of this volume is to give an overview of computational chemistry in a broad sense, from *ab-initio* quantum chemistry via semiempirical MO theory and molecular modelling to the use of databases for three-dimensional structures. A reader working in one of these different branches of computational chemistry is invited to learn at least the basic features of other branches, which may promote communication that has so far been inhibited by misconceptions such as that 'molecular modelling' is simple-minded or that *ab-initio* theory is of no practical use.

From the field of *ab-initio* theory there is thorough discussion of basis sets by D. Feller and E. R. Davidson (Chap. 1), a presentation of the 'direct' calculation of properties, especially energy derivatives by C. E. Dykstra, J. D. Augspurger, B. Kirtman, and D. J. Malik (Chap. 3) and some sceptical but lucid comments on *ab-initio* calculations by E. R. Davidson (Chap. 11).

The semiempirical approach is treated by J. J. P. Stewart (Chap. 2) with respect to the history of CNDO-like methods, culminating in MNDO, AM1 and PM3. The basis aspects of molecular modelling are reviewed by D. B. Boyd (Chap. 9), who also wrote a useful appendix on available software for molecular modelling.

Examples of computer-assisted molecular design are discussed in Chap. 10 by D. B. Boyd on a general level and in Chap. 4 by E. L. Plummer for the special case of pesticides. Biological applications are described in Chap. 8 by T. P. Lybrand.

Methods making use of databases are the subject of Chap. 6 by Y. C. Martin, M. G. Bure, and P. Willet, chemometrics and multivariant analysis in analytical chemistry are reviewed by P. C. Jurs (Chap. 5), while P. G. Mezey's chapter on molecular surfaces (Chap. 7) is somewhat independent of the hierarchy of approximation methods.

Most chapters contain an extensive bibliography that allows one to trace back the most important original literature.

One may regret that the stress on computation excludes those parts of theoretical chemistry that are not or only marginally computational.

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K. B. Lipkowitz, D. B. Boyd (eds) Reviews in Computational Chemistry. Vol. 2. VC, Weinheim, 1991, 527 pages, 91 figures, 54 tables, DM 236

This second volume of the series follows the concept of the first one to assemble under one cover review papers on computational chemistry from the most sophisticated to the most simple-minded approaches. On the *ab-initio* side there is a rather extensive review by S. Scheiner on hydrogen bonds (Chap. 5). Based on *ab-initio* theory are the molecular electrostatic potentials presented by P. Politzer and J. S. Murray (Chap. 7) and the related net-atomic-charge and multipole models reviewed by D. E. Williams (Chap. 6).

M. C. Zerner's contribution on semiempirical molecular orbital methods (Chap. 8) can be regarded as the advanced counterpart to J. J. P. Stewart's review in Vol. 1. Two chapters are devoted to the force field approach, one (Chap. 3) by J. P. Bowen and N. L. Allinger, the other (Chap. 4) by U. Dinur and A. T. Hagler. Both are concerned with the parametrization of force fields, the latter chapter devoting itself to the interesting problem of how to derive force fields from *ab-initio* data.

Chapter 1 by A. R. Leach is a general study of conformational search. Two chapters, one (Chap. 9) by L. H. Hall and L. B. Kier and the other (Chap. 10) by I. B. Bersuker and A. S.

Dimoglo, deal with the QSAR (quantitative structure activity relation) approach. The former chapter concentrates on 'chi indices' and 'kappa-shape' indices. Simplified models for protein structures are discussed by J. M. Troyer and F. E. Cohen in Chap. 2.

The book ends with a chapter by D. B. Boyd on the computational chemistry literature. The author and coeditor cannot resist the temptation to consider the conclusions drawn from the Science Citation Index. One would welcome this, if it were meant as a curiosity and if the chance had been taken to demonstrate how little reaction there is between the number of quotations and the importance of a scientific paper. Unfortunately this is taken seriously and this gives the volume a dubious touch.

Nevertheless, like Vol. 1, this book (including the appendix on available software packages) is a good source of information and references and should serve as a basis for communication between computational chemists on different levels.

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