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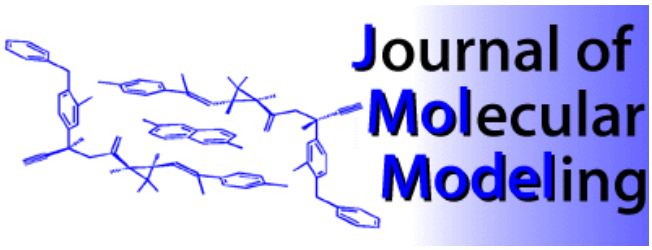

Book review

Reviews in Computational Chemistry, Volume 10

Edited by K.B. Lipkowitz and D.B. Boyd, VCH Publishers, New York, 1997. ISBN 1-56081-957-X. US $ 120.–

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A review of the tenth volume of the *Reviews in Computational Chemistry* must be taken in the context of the other nine. Since the first volume, which was published in 1990, the editors K.B. Lipkowitz and D.B. Boyd have succeeded in bringing together reviews by the leading scientists in computational chemistry. The editors always urged the authors to present their research in a clear and understandable way. This makes the reviews both an excellent source of information for students as well as for scientists working in the field. The *Reviews in Computational Chemistry* are definitely a must for everyone working in computational chemistry.

The first review, written by Richard Judson is on genetic algorithms and their use in chemistry. After a general outlook on what genetic algorithms are and why they work, the author gives a review of the large range of chemical applications that use genetic algorithms. He focuses on their use for global optimization, e.g. in conformational searching and data fitting. The chapter closes with suggestions for further reading and for public domain genetic algorithm source codes.

In the next review, Eric J. Martin, David C. Spellmeyer, Roger E. Critchlow Jr., and Jeffrey M. Blaney raise the interesting question: "Does combinatorial chemistry obviate computer-aided drug design?" The authors answer clearly that it does not. They demonstrate how methods developed for computer-aided drug design can support combinatorial chemistry. Computational methods allow the efficient design of experiments ensuring either maximum diversity of a combinatorial library or bias of the library for a particular biological target.

Reviews 3 and 4 survey new developments in the area of non-linear dynamics. Robert Q. Topper explains new developments in the theory of molecular reaction dynamics and emphasizes the importance of non-linear effects on the dynamics of elementary reaction steps.

A different aspect of non-linear dynamics is covered by Raima Larter and Kenneth Showalter. They describe the interesting phenomena appearing in complex reaction systems. If non-linear effects become important, temporal and/or spatial patterns or even chaotic behaviour can occur.

A description of "the developement of computational chemistry in the United Kingdom" finally closes this tenth edition. The historical look back of the authors Stephen J. Smith and Brian T. Sutcliffe is very lively and interesting to read.

Again, the editors present a collection of well written and very informative reviews. But, a drop of bitterness remains; the price of $ 120.– is very high.

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