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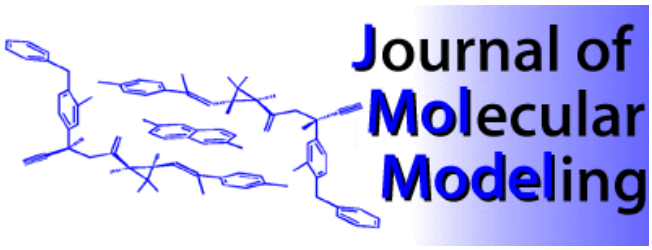

Book review

Reviews in Computational Chemistry, Vol. 8

Edited by K.B. Lipkowitz and D.B. Boyd, VCH Publishers, New York, 1996. ISBN 1-56081-929-4. US $ 110.–

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In the preface, editors K.B. Lipkowitz and D.B. Boyd raise the question "How widely used is computational chemistry?". In answer, they report a literature database survey, confirming the growing importance of computational chemistry in all subdisciplines of chemistry.

The eigth volume of this series covers on the one hand theoretical studies of large molecules, on the other hand computational methods to treat heavy elements.

The first chapter is about fullerenes. Zdenek Slanina, Shyi-Long Lee, and Chin-hui Yu describe this flourishing, exciting new field of carbon clusters. First, they demonstrate the limitations of standard semi-empirical methods and show how they can be reparameterized to reproduce experimental data correctly. Next, the whole range from *ab-initio* calculations of small carben clusters to semi-empirical treatments of higher fullerenes is covered.

The next two chapters deal with *ab-initio* methods using effective core potentials. The first by Gernot Frenking and co-workers describes the application and accuracy of such pseudopotential calculations for transition metal compounds. The selected examples include organometallic complexes, like carbonyl or carbene complexes, as well as catalytically important oxo and nitrido complexes.

The third chapter, written by Thomas R. Cundari, Michael T. Benson, M. Leigh Lutz, and Shaun O. Sommerer, gives some insight in how effective core potential functions are derived. The following examples cover main group chemistry as well as transition metal and lanthanide chemistry.

The fourth chapter reviews the current methods to include relativistic effects in computational chemistry. These effects are of great importance for heavier elements. Although this topic requires a profound theoretical background, the authors, the late Jan Almlöf and Odd Gropen, succeed in making it relatively easy to understand.

In the final chapter, Donald B. Chesnut reviews *ab-initio* computation of NMR chemical shifts. First, he describes the theoretical basis on a non-expert level and discusses the quality of the calculations. Then, he gives several examples. Here, he not only reviews some calculations of rather small molecules, but also describes how NMR calculations can be applied to gain more insight in the NMR properties of larger systems, like proteins or water. The chapter closes with a discussion of the importance of correlation effects.

Again, the editors have achieved their goal to provide 'tutorials and reviews for both novice and experienced computational chemists'. Unfortunately, the high price of this book will prevent wide distribution among students, and considering the tight financial situation at universities maybe even there.

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