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Book Review

Jonathan M. Goodman, *Chemical Applications of Molecular Modelling* (ISBN 0-85404-579-1), xv + 216 pp., The Royal Society of Chemistry, Cambridge, 1998, £25.00.

Molecular Modelling is of rapidly growing importance in modern chemistry in areas such as drug design, structural biology or supramolecular chemistry. Goodman's book is a basic introduction to the field for both students and experimental organic chemists and is by no means written for "theoreticians" and researchers with a profound background in computational studies of chemical processes and structures. A brief introductory chapter is followed by an explanation of force fields and their different energy terms. Next is a description of the principles of energy minimization and some common available algorithms. Conformation searching by different procedures such as Monte Carlo search or genetic algorithm as well as molecular dynamics calculations are crucial steps in molecular mechanics studies and accordingly one chapter each attends to the explanation of these methods. Chapter six is an introduction to the basics of molecular orbital theory including a comparison between ab initio calculations and semi-empirical methods. The book closes with a brief description of database searching and a series of examples of molecular modelling calculations taken from the literature, namely structure and transition state calculations as well as drug design. Finally there is a glossary with "all those abbreviations" typically found in publications and an appendix listing physical constants, force fields, "useful mathematics", and more, as well as recommendations for further reading. Additionally, the chapters about minimization, conformation search, and MO theory have extended subchapters with numerous questions and tasks, the answers and results of which may be calculated with any commonly available modelling program and are then discussed in detail. This way the reader can immediately apply what he just learned.

The book is consistently "very easily readable" and never overwhelms the reader with dry theory; it avoids where possible mathematical discussions in order not to scare away the novice and does not use phraseology that can only be understood when already having deeper insight. The aim of the author to "demystify molecular modelling and enable the non-specialist to appreciate the power, but also the limitations, of the computational tools available" – to cite the cover text

– is fully achieved. In times where MM calculations are of increasing importance but its principles still are not part of every chemistry student's curriculum, this is a very useful monograph both for autodidactical purposes and as a base for a teacher's preparation of a course on this topic. *Chemical Applications of Molecular Modelling* is highly recommended and should not be missing in the library of any chemistry department. It would make a useful addition to every organic chemist's text book collection.

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