

## Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.*

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**Molecular modeling of inorganic compounds.** Edited by P. COMBA AND T. W. HAMBLEY. Pp. x + 197. Weinheim: VCH Verlagsgesellschaft mbH, 1995. Price DM 197.00. ISBN 3-527-29076-1.

Traditionally, molecular mechanics methods have been associated with the calculation of the structures of organic molecules. Application of these methods to inorganic compounds has been hampered by several obstacles, including problems with parameterization and the varied coordination geometries of metal ions. However, in recent years, several reviews have pointed to new and exciting developments in overcoming these obstacles and this book provides the reader with a broad overview of the current state of molecular modeling for inorganic systems. Both authors are experienced workers in the field of molecular mechanics as applied to metal complexes and this monograph focuses on that method, leaving out other areas of computational chemistry such as quantum chemistry. A concise but informative introduction is followed by three major parts. Part I, devoted to the theory of molecular modeling, reviews in detail such fundamentals as potential energy functions and force-field parameters. The authors characterize the force fields used in coordination complexes and compare them with those applied to organic compounds. Limits in applications are carefully discussed and there are frequent calls for caution in the interpretation of results. I consider this one of the main strengths of the book; it is all too easy to forget these limitations when working on computers equipped with powerful molecular graphics routines, where the beauty of the image may all too often be mistaken for reality. Part II, describing applications, constitutes the central core of the monograph and it is here that the real status of the field is revealed. Numerous examples, many taken from the authors' own work, illustrate the successes of molecular mechanics applied to the structure, stereoselectivity, spectroscopy and mechanistic aspects of coordination, organometallic and bioinorganic compounds. The best accuracy has so far been achieved for a variety of amine complexes of the first-row transition metal ions. Reasonable models have also been developed for alkali and *alkaline earth metal complexes with crown ethers, cryptands, spherands and some ionophores and cyclic antibiotics, and p-block elements are modeled relatively readily.* However, the complexity and size of metalloproteins and nucleic acid-metal assemblies, as well as the lack of clearly defined atomic connectivities and bond types in most organometallic compounds, still seem too prohibitive for these systems to be handled with any confidence. Part III is a short section on the practice of molecular mechanics involving metal complexes. Some practical aspects of force-field development and general procedures for carrying out the calculations are presented. The authors carefully evaluate the design of appropriate force-

field terms, indicating the need for experimental data of good quality. I believe that many beginners, however, would benefit from a more detailed treatment of the interpretation of results than that presented in the final chapter. This book should be read by everyone with an interest in the molecular modeling of inorganic systems. It is full of excellent practical hints that can enrich the computational skills and awareness of both the novice and the more experienced user. It also has its share of typographical errors and the quality of some drawings, especially those illustrating the structures under discussion, could be improved. However, these defects aside, I believe that the authors have achieved the important goal of presenting the state of the art in this rapidly developing field.

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### Books Received

*The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.*

**Fundamental principles of molecular modeling.** By W. GANS, A. AMANN & J. C. A. BOEYENS. Pp. viii + 249. New York: Plenum Publishing Corporation, 1996. Price \$79.50. ISBN 0-306-45305-3.

This volume contains the proceedings of the 'Small Molecules Indaba' devoted to the title topic, an international workshop organized by the South African Crystallographic Society in collaboration with the Small Molecules Commission of the IUCr, held at Skukuza, Kruger Park, South Africa in August 1995. In a generally cautionary introductory presentation, Professor Boeyens offers the following eight propositions, at least some of which should stimulate useful lunchtime discussion: (i) There is no proof that an isolated molecule has a rigid characteristic shape. (ii) It is not possible to determine the structure of a molecule in the gas phase or in solution. (iii) The three-dimensional Fourier transform of crystallography does not necessarily contain the full translational symmetry of a crystal. (iv) The *R* factor of a crystallographic analysis is not the only measure of the reliability of a reported struc-

ture. (v) Crystallographic standard deviations are a measure of internal consistency only and not an absolute measure. (vi) Undetected disorder can be mistaken for unusual molecular conformations in the absence of independent molecular

modelling. (vii) Molecular structures and shapes cannot be predicted or calculated by quantum mechanics. (viii) Deformation densities are not an objective representation of the electronic effects of chemical bonding.