Molecular Modeling of Inorganic Compounds
Peter Comba and Trevor W. Hambley
VCH, Weinheim, 1995
240 pp. £76.00
ISBN 3-527-29076-1

The claim that this book will be invaluable for everyone working in or entering the field of quantitative atomistic-based modelling of inorganic compounds is not far from the truth. An experimental inorganic chemist would have to be exceptional to enter the field solely on the basis of this book plus whatever software seemed appropriate, but most graduate students would find it invaluable for avoiding the common pitfalls as well as writing up the introductory sections of their theses.

The book has three sections: Part I, Theory; Part II, Applications; and Part III, The Practice of Molecular Mechanics, as well as various appendices including a listing of various software and force-fields. The theory section deals with parameterization, generalizing well over the various force-fields and making it clear that molecular mechanics is an interpolative procedure. The sections on various minimization methods and the multiple-minima problems are also good for their emphasis on the limitations and possible problems of such methods, and form a good antidote to the hype that can be associated with commercial modelling packages. An expert on each section could well criticize the level of coverage afforded in less than 50 pages for Part I, but this is compensated for by over 100 references.

The applications section is very wide ranging, covering structural aspects, stereoselectivities, metal-ion selectivity, spectroscopy, electron transfer, electronic effects, bio-inorganic chemistry, organometallics, and compounds with *s*-, *p*- and *f*-block elements. A good grasp of the underlying inorganic chemistry is assumed, and so the main emphasis is on reporting the results and commenting critically on the approximations made. This is often quite incisive, and the theme that 'the quality of the force-field parameters depends on good fitting of carefully chosen experimental data, and that they are not necessarily related to physically meaningful parameters' is well established. In some more peripheral areas the coverage is rather superficial and degenerates to almost a mere listing of what has been tried on which systems. Nearly 300 references, almost 40% originating in 1990 or later, provide the entry point to most of the fields, which again, in less than 100 pages, are generally given the sort of treatment that will be useful to those in adjacent areas, but may not please all who specialize in a specific application.

The final 20-page section of practical advice on how to apply molecular mechanics to problems involving metal complexes, and how to interpret and use the results, does indeed highlight many of the common pitfalls. Nevertheless, the overall tone of the book is optimistic, and many will be interested and pleased to see how well molecular modelling can perform for carefully chosen problems, even when electronic effects are important.

This book may date more rapidly than similar books in equivalently lively research fields, because molecular mechanics methods fundamentally have to approximate electronic effects (e.g. Jahn–Teller distortions) which tend to be more important in inorganic than organic problems, a theme which is well treated in this book. State-of-the-art studies of many areas of inorganic chemistry may soon be based on quantum mechanics rather than molecular modelling, given recent advances in computer power and in computational methods which treat the electrons explicitly. However, this book is well timed for the many who want to complement their experimental ligand design work with some modelling calculations, and will provide a benchmark for the evolving quantum methods.

The book will be a great help for graduate students in the area, and provide food for thought for the experts. However, although most sections would represent a very high level of doctoral thesis, benefiting from the authors' evident maturity in the field, there are a disconcerting number of typographical errors, equations poorly or inconsistently defined, and other signs of a rushed production that would not impress most PhD examiners. The price, £76, means that the book's most avid users are unlikely to buy their own copies.

SARAH L. PRICE
University College London

 CCC 0268–2605/97/050457–02 $17.50