



A Practical Introduction to the Simulation of Molecular Systems, *M.J. Field*, Cambridge University Press, 1999, pp: x+325, ISBN 052158129X (hc); Price: US\$80.

The determination of the spatial structure of molecules has always been of central interest to chemists. Until very recently, the only generally applicable method has been X-ray Fourier analysis, and that too has suffered from the absence of phase information in normal diffraction spectra. In some special cases this deficiency can be overcome by such things as the use of heavy-element variants or lattice expansion as in the classical work of Bragg and Perutz: but this is unusual.

After the advent of electronic computers in the late 1940's, their further development was spurred by the need to determine structures directly via minimization algorithms. However, limitations of the machines (4096 words of high-speed memory and addition times of 1 microsecond) prevented their use for the mathematical techniques that were being developed. Only in the last few years have computers become sufficiently powerful to allow these techniques to be applied to substantial problems of interest.

Field's book does several things: It describes DYNAMO, a special library of routines for simulation developed at the University of Grenoble; it provides a systematic method for the use of this library; and it supplies both worked examples of the use of simulation techniques, and examples for the student. In addition, the theoretical bases of most of the available minimization targets are discussed.

Of special interest are Chapters 6 and 7, which discuss the difficulties resulting from the presence of maxima, minima, and saddle points in the minimization field; these cause most methods to require special external assistance. Actual outputs are illustrated from the cyclohexane molecule for which a number of possible configurations have to be resolved.

There are twelve chapters in the main part of the book and an appendix describing the DYNAMO library. There is also an excellent nineteen-page bibliography, an author index, and a subject index.

All of the exercises and examples are available from the Grenoble website,¹ as is the complete DYNAMO library. There is only one snag — the code is written in FORTRAN 90, a language for which compilers are not generally available on small machines.² This is a pity because the latest generations of desktop computers are suitable for small example problems. Will some group eventually convert the code to the more common C++ language?

A Practical Introduction to the Simulation of Molecular Systems is a splendid book, useful both as a teaching tool and as a research handbook.

Andrew D. Booth
Sooke, British Columbia, Canada

1. http://www.ibs.fr/ext/labos/LDM/projet6/welcome_fr.htm

2. A comprehensive list of Fortran 90 and Fortran 95 resources, including free compilers for Linux, Windows, and the Macintosh, is at <http://www.fortran.com/fortran/metcalfe.htm>. -Ed.(BR)