book review

Computer Simulation of Polymers

R. J. Roe (Ed.)
Prentice-Hall, New York, 1991, 404 pages, £74.90
ISBN 0-13-161480-0

In recent years there has been a tremendous growth of activity in the area of computer modelling of materials in general and synthetic polymers in particular. This has not been confined to the calculation of polymer molecular configuration but also includes organization into supramolecular entities, crystalline organization and property prediction. The demand to be able to calculate such properties of polymers has always been there and it is the huge increase in computing power available at prices which are in the realms of possibility for research institutions and academic institutions which has fuelled the increased activity in software production. Not so many years ago, calculations which can now be done (and visualized) on a desk top high resolution graphics work station were only possible using high power mainframe computers usually only available at regional computing centres. Nowadays more and more research groups are acquiring the necessary hardware and the (commercial) software to enable modelling of polymer systems. It may be that such modelling will be a major growth area in polymer research in the future. After all, it will be cheaper to model and predict the properties of putative molecules rather than invest in production of sufficient quantities to evaluate the properties which you then find do not fulfil the requirements! With all the computing power available and the versatility of the software, the combination of which provides some very impressive graphics, the users must keep reminding themselves that the software is based on theories which may have a less than total relation to the scientific truth. This is not a criticism of the software or the writers of the programs but merely a warning that users should keep their scientific feet on the ground. From the point of view of the non-expert who uses computer simulation packages, what is needed is a discussion of the various theoretical methods, the approaches used, an objective discussion of the limitations and perhaps most importantly a comparison of computer predictions with experiment. This book does not fulfil all of the objectives listed above but it does address some of them (notably there is a liberal sprinkling of real data) and it certainly displays the breadth of application of computer simulation to polymers. There are 28 separate contributions to the volume and they constitute the papers given at a five day symposium, with the same title as the book, in 1989 sponsored by the Polymer Chemistry Division of the American Chemical Society. The subjects covered include *ab initio* quantum chemical methods to calculate intramolecular rotational potential energy functions, the simulation of glassy polymers at interfaces, diffusion behaviour of polymers and small molecules in polymers, nematic liquid crystals, spinodal decomposition and the application of scaling concepts to phase behaviour. Within this broad scope, the variety of methods used in the computer simulations encompasses almost all of the currently fashionable approaches; use of MNDO and AM1 packages, Monte Carlo methods, molecular dynamics, analytical solution of Langevin equations with numerical evaluation and renormalization group methods. All are written by acknowledged experts (Mattice, Warner, Stepto, Kremer and Olvera de la Cruz are amongst the authors) in the various areas and the articles vary in length and depth. None is suitable for the beginner in the field. Nevertheless this book should eventually end up on the shelves of those who are seriously interested in using computers to simulate polymers and their properties and should certainly be in the library of any institution which has any involvement in the field of computer modelling at all.

For beginners and novices, very useful introductions to various aspects of computer simulation can be obtained from the books by Hirst ('A Computational Approach to Chemistry'), Allen and Tildesley ('Computer Simulation of Liquids') and of course Flory's 'New Testament' ('Statistical Mechanics of Chain Molecules'). A 'how to' description of semi-empirical quantum mechanical programs as implemented in the MOPAC package has also been provided by Stewart (*J. Comp. Aided Mol. Design* 1990, **4**, 1). A look at some of these would be of value before picking up the book reviewed here.

R. W. Richards
IRC in Polymer Science
University of Durham

0032-3861/93/061342-01