

## NEWS

## Book reviews

**Molecular Mechanics across Chemistry**

by A. K. Pappé and C. J. Casewit, (University Science Books, 1996)  
ISBN 0 935702 77 6, 444 pp

Increasingly, industrial researchers are having to tailor new products to meet specific requirements, and to deliver them to the marketplace as quickly as possible. Molecular mechanics now plays a significant role in meeting these challenges by helping scientists to understand products and processes at the atomic level. Besides increasing our fundamental understanding of molecules, molecular mechanics calculations are routinely employed to predict a range of properties and have, hence, become an integral part of modern day chemistry. As a result of this, many chemistry departments have now introduced the subject into their courses. However, very few textbooks are specifically designed for advanced undergraduates, postgraduates and newcomers to the field; this is precisely the readership that the authors aim to reach.

To survey the use of molecular mechanics in chemistry is a tremendous undertaking; there is a broad spectrum of applications and it is becoming increasingly difficult to keep up with the latest developments. In this book Pappé and Casewit satisfy the needs of both experts and casual observers by giving an excellent overview of the subject.

Rather than providing a comprehensive review of the vast array of problems currently being addressed with the aid of molecular mechanics, a case study approach is adopted. This exposes the reader to the relevance and utility of molecular mechanics while offering the opportunity to consider the molecular mechanics solution to a particular chemical problem. At the end of each of the eight chapters there is a selection of problems designed to familiarize the reader with the conventional thinking and method applied in tackling such problems; the only requirement is that the reader has a solid background in chemistry, physics and mathematics.

**Electrosíntesis y Electrodiálisis: Fundamentos, Aplicaciones Tecnológicas y Tendencias (in Spanish)**

by J. R. Ochoa, (McGraw-Hill, Madrid, 1996)  
ISBN 84 481 0389 0, 337 pp

This book fills a gap in the Spanish literature on industrial electrochemical technology, only previously covered by Coeuret's text, 'Introducción a la Ingeniería Electroquímica' (Reverté, Barcelona, 1992). Ochoa provides a brief explanation on fundamental concepts on electrochemical technology and a description of those components found in electrochemical reactors. The contents include descriptions

In Chapter 1, the development of molecular mechanics and conformation analysis is presented by combining an historical perspective with a conceptual development approach. In the second chapter, the basic theory employed for the determination and interpretation of preferred molecular conformations, transition state structures and the intermolecular energetics of organic systems are explained and discussed. Chapters 3 to 5 concentrate on the study of the interaction of biomolecules with drugs: Chapter 3 concentrates on peptides and proteins, Chapter 4 deals with drug design whereas Chapter 5 focuses on the study of DNA. The aim of Chapter 6 is to present a flavour of the many possible applications of molecular modelling to the study of polymeric materials. Inorganic materials are considered in Chapter 7. The final chapter presents the augmentation and design of new force fields. Several useful appendices provide descriptions of stereochemical terminology, ideal gas thermodynamics, molecular dynamics, Monte Carlo selection procedures and conformational searching techniques. The answers to selected problems, from those presented at the end of each chapter, are also appended here.

The book is nicely produced, well referenced and there are many illustrations and tables to present useful information concisely. The text and the figures are clear, concise and remarkably free from inauspicious errors. The authors have taken great care to introduce the complexities of the subject progressively. The writing style is user-friendly, as is the substantial index. Considering the wealth of information it puts at your fingertips, this book is excellent value for money. Although I would not go as far as to suggest that this book should feature on every chemists bookshelf, it would certainly be a useful addition to any institutional library.

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of electrode materials, membranes, turbulence promoters and commercially available cells. A mathematical treatment has been avoided in order to make the text more readable. Industrial examples of electrosynthesis and electrodiálisis are treated in separate chapters which include extensive information on industrial processes. Process operational conditions, economics and figures of merit provide a useful means of comparison of reported electrochemical processes with competing technologies.

The text is illustrated with plates supplied by electrochemical hardware suppliers from Europe and the United States of America. Technical data for

some of the products and the addresses of the suppliers are helpfully provided. Because of the avoidance of a mathematical treatment and no requisite previous knowledge of electrochemistry, the text is easily accessible to a wider scientific audience. The reported industrial applications allow the reader to appreciate the usefulness of electrochemical techniques to industrial problems.

This book has been sponsored by two Spanish utility companies and, as such, it provides a good

example of collaboration between university and industry regarding basic research and educational material. Undoubtedly, as a reference text and sourcebook, this will be a significant contribution to electrochemical technology in Spanish speaking countries.

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