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### Book Reviews

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## Book reviews

*Dynamics of Proteins and Nucleic Acids.* By J. ANDREW MCCAMMON and STEPHEN C. HARVEY. (Cambridge University Press, 1987.) [Pp. 234.] ISBN 0 521 307503.

In the last thirty years there has been a revolution in our knowledge of biological molecular structure, brought about by the X-ray analysis of hundreds of proteins and nucleic acid molecules at close to atomic resolution. The architectural forms and geometrical principles of protein structure are by now well described and understood in general terms. The atomic positions have also shown us the mechanisms of essential protein functions, such as the binding of oxygen by haemoglobin or the catalytic activity of enzymes. Nucleic acid structures known today range in scale from small segments of double-helical DNA to transfer RNA and large solenoidal nucleosome core components. Recent work on the complexes of DNA with repressor and operator proteins is beginning to reveal the switching processes that control gene activity.

At a deeper level, beyond architecture and simple chemistry, lies the need to understand the processes that fold and assemble the structures of living molecules, and in particular to discover how their amino acid or nucleic acid sequences lead to the formation of a unique native structure in the cell. A new theoretical science, classical dynamics of very large molecules, has developed during the last ten years; its object is to answer these questions by computer simulation of actual atomic motions in a protein or nucleic acid molecule. This work followed on the realisation that conformational energy calculations themselves will never give an answer, because they do not allow either for thermal motion or for the effects of surrounding water and dissolved ions inside the cell.

McCammon and Harvey's book is the first full-scale account of this new discipline, written with enthusiasm and a firm grasp of detail by two of the leading exponents of the method. Their book is easy to read and is simply presented. A graduate student should easily be able to follow the very simplified mathematics and to understand the gist of the ingenious techniques that are used to extract scientific meaning from a few hundred picoseconds of molecular motion. There are plenty of references to all the basic ideas and techniques, while a minimal sketch of protein and nucleic acid structural principles is included to help the beginner.

The book explains how the most successful applications of dynamical simulations so far are over short time periods of about 10–100 picoseconds. One can thereby account nicely for the crystal cell temperature factors of amino acid side chains in enzymes—the vibrations of atoms about their stable mean positions—and explore other short term motions; the partial unfoldings of a protein surface that allow hydrogen-bonded protons to exchange or that let oxygen diffuse into the haem pocket of haemoglobin are good examples. Low-frequency vibrational modes are studied profitably to examine the flexibility of small proteins. In DNA the atomic trajectories help to show how distortions and untwisting can change the structure of the double helix. McCammon and Harvey also take us through some of the more difficult and ambitious applications: the hinge bending of the lysozyme active centre; the benzene ring flipping of a tyrosine side chain in a trypsin inhibitor from cow pancreas. These two examples show nicely how the techniques of dynamics can be tailored for special investigations. They also serve to warn us that simulations are still relatively crude and numerically inaccurate. Wuthrich and Baumann analysed the carbon-13 NMR spectrum of this inhibitor tyrosine and found the ring to be immobile for a time of at least 5000 picoseconds, significantly longer than dynamic estimates. However the dynamics techniques are improving rapidly and should graduate from pioneering exploration to reliable maturity during the next decade.

I hoped that the authors would provide a more deeply founded, even if brief, guide to the fundamental principles of dynamic simulation, so that a novice like myself would feel ready to go to his computer and write some simple programs. This book is more like a giant-sized review article full of interesting pointers to follow up. I would like to see deeper discussion of the differences between Monte Carlo and dynamics methods; more explanation of the tantalisingly short appendix on numerical construction of the trajectories; a well-rounded treatment of normal mode theory and autocorrelation functions. For the molecular specialist, I would like to see some critical analysis and discussion of potential energy functions and their numerical values,

with guidance about their validity; really good clear diagrams of the internationally recognized angles used to describe protein and DNA structures would also be helpful.

This book is a valuable guide to the field and will lead to a wider appreciation of how these new computational methods can help us to understand molecules at work in the living cell.

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*Nuclear Magnetic Resonance, Volume 17, Royal Society of Chemistry Specialist Periodical Reports. Senior Reporter: G. A. WEBB (Royal Society of Chemistry, 1988.) [Pp. 481.] £110.00. ISBN 0 85186 402 3.*

This volume, in the Royal Society of Chemistry's valuable Specialist Periodical Reports series, covers the topic of nuclear magnetic resonance spectroscopy as represented in the published literature between June 1986 to May 1987. As is usual with these reports, sections covering the various topics are contributed by different authors each of whom is judged to be an authority in that field. The topics considered cover the whole range from theoretical calculations of NMR parameters to studies of amorphous solids, and reading the volume certainly does convey a sense of the incredibly wide range of systems that are studied by NMR spectroscopy.

The various chapters fall into two broad categories. Those chapters covering areas that are now almost a matter of routine are little more than a list of literature references, carefully sorted by subject. These chapters do not attempt any critical appraisal and could perhaps be more conveniently condensed into tables and indeed on occasion some of the reporters adopt this approach. However, in the very wide areas covered by these sections, it would certainly be almost impossible for one person to be able to make an informed critical evaluation.

The second type of chapter are those which attempt a much more critical evaluation of the literature, all be it generally in an area where the amount of reported literature is much less. Some of the reporters are clearly promoting their particular view of certain, presumably controversial, topics and in some cases an almost crusading zeal is displayed. However, on the whole these sections seem to be reasonably balanced and provide a useful guide for non-specialists.

The report covers a very wide range of literature, including many non-English language publications and there is a separate listing of reviews and books which is most welcome. The presentation is clear and the use of camera-ready copy should result in as few transcription errors as is possible for such a formidable undertaking. There is a certain amount of overlap between some of the sections, but this seems to have been kept to a reasonable level, no doubt due to a firm guiding hand from the senior reporter.

This report contains chapters dealing with the basic NMR phenomena of nuclear shielding, spin-spin coupling and relaxation. Both theoretical and experimental applications of nuclear shielding are discussed, but spin-spin coupling is only discussed from a theoretical stand-point (an omission to be remedied in the next volume). Solid-state NMR is treated in a separate section and also appears in an extensive chapter concerned with applications to heterogeneous systems, such as zeolites. A section devoted to the ever burgeoning field of technical multiple pulse NMR brings a welcome note of order into this untidy area. Conformational analysis, mostly of medium-sized organic and inorganic molecules, is the subject of a further section and macromolecules of both natural and synthetic origins are treated as separate topics. A chapter is devoted to the NMR of oriented molecules and, resting somewhat uncomfortably along the heavily chemical emphasis of the rest of the volume, is a section covering NMR imaging and the NMR of living systems.

This volume represents a very considerable effort on the part of the reporters, and is an invaluable guide to the NMR literature that should be found on the shelves of a well-stocked library.

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*Advances in Boron and the Boranes*. Edited by J. F. LIEBMAN, A. GREENBERG and R. E. WILLIAMS. (VCH, 1988.) [Pp. 547.] DM 195. ISBN 0 89573 272 6.

*Advances in Boron and the Boranes* is a volume in a series of books following a theme of 'Molecular Structure and Energetics'. This particular volume is a collection of essays dedicated to Anton B. Burg. The first chapter, by Burg himself, is a lively, historical account of the pioneering days of Lewis base-borane chemistry. The remaining 21 chapters span structural, physical, theoretical and synthetic aspects of borane, carborane, metallaborane, metallacarborane and organoborane chemistry. The book's great strength lies in the fact that it takes an overview of a large field; not so much a comprehensive survey, as a whetting of the appetite through the eyes of boron chemists. Several authors have chosen to review their area of chemistry, while others have concentrated on a detailed (usually with up to the minute results), account of a specialized topic.

Taking each chapter in turn, we begin with the chemistry of pentaborane (9) (Shore *et al.*); traditional borane cage reactions are described along with some new and novel metallaborane cluster chemistry. A review of 9- and 10-atom carboranes and heteroboranes by Stibr *et al.* follows. Sneddon *et al.* have described some intriguing cage-coupling reactions in a chapter which focuses on palladium- and platinum-promoted reactions of boranes and carboranes. Some elegant mechanistic studies emphasizing the usefulness of boron isotopic labelling are detailed by Gaines *et al.* A direct link with Burg comes in the chapter by Kodama, in which trimethylphosphine boranes are proven to be anything but *just* Lewis base adducts! Onak has chosen to focus upon one aspect of carborane chemistry: the effect of substituents on cage structure. Morrison provides a balanced historical/contemporary overview of the chemistry of polyhedral boron halides, which ends with a timely 'where shall we go from here?' The extent to which carbocations may be considered to be nonclassical and borane-like is examined in a chapter by Williams *et al.*; correlations between  $^{11}\text{B}$  and  $^{13}\text{C}$  NMR data provide the best evidence for a carbon/boron bonding analogy.

Metallaboranes form a common theme for the next few chapters. Hawthorne describes recent research which addresses the catalytic activity (or not) of icosahedral metallacarboranes. An important chapter by Grimes points out that, while serendipitous syntheses have certainly provided boron chemists with a wealth of novel compounds in the past, it is high time we spent some time developing rational synthetic pathways. Ingenuity is the keyword, and Grimes certainly illustrates some elegant ways of controlling reactions. The versatility of monoborane is expressed in an account by Fehlner; the question: 'does monoborane "remember" its parentage once attached to a metal?' is examined. Heteroatom incorporation into borane clusters is described, first in a chapter concerning thiaboranes and azaboranes (Todd *et al.*), and also in an account of heterocarboranes containing Al, Ga, Si, Sn or Ge atoms (by Hosmane *et al.*). The area of boron neutron capture therapy is of growing interest and is represented in a section by Spielvogel on boron compounds of relevance to the medical world.

Three chapters follow which change the pace of the book. Organoborane chemistry, despite being a vast field, is given a brief airing in this book. This is probably a suitable choice by the editors, and Matteson provides an interesting chapter on the use of boronic esters in chiral synthesis. An overview of the chemistry of pyrazaboles (Niedenzu) is a useful addition to the book, given that these compounds are frequently exploited as ligands in transition metal chemistry. The chapter by Siedle describes organometallic chemistry of fluorocarbon acids. While most certainly appropriate as a tribute to Anton Burg, this account does not fall under the book's title of 'Advances in Boron and Boranes'. Back to boranes, and Bauer provides a review of the gas-phase kinetics of boron and small borane molecules which compliments the first part of the chapter by Fehlner. Beaudet's contribution to the book provides a timely review of borane and carborane structures; the appendix of coordinates is a valuable compilation in these days of readily accessible computer graphics.

One of the editors, Liebman, has co-authored a chapter which introduces 'plemeioelectronic' relationships between geometrically similar, but non-isoelectronic, species. Empirical methods of predicting thermodynamic quantities are explored with some useful results. A contribution by Linus Pauling *et al.* concludes the tributes to Burg; this is an interesting assessment of the place of the unsynchronized-resonating-covalent-bond theory as a means of explaining the bonding in elemental boron and boranes.

In summary, I would say that this book should find its way into the collections of most boron chemists, and will be an asset to academic libraries. Reading the varied essays certainly gives one the feel that boron chemistry has come a long way in recent years... and still has far to go.

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*ICORS London 1988: International Conference on Raman Spectroscopy*. Edited by R. J. H. CLARK and D. A. LONG. (John Wiley & Sons, Chichester, 1988.) [Pp. liv + 1034.] £60. ISBN 0 471 92094 0.

The vibrational spectroscopies have achieved a major renaissance over the past decade: the family of infrared spectroscopies, largely through the widespread application of Fourier-transform techniques, and the family of Raman spectroscopies through the use of lasers.

As its title implies, this volume contains the proceedings of what was a highly successful Raman spectroscopy conference held in London in 1988. It contains abbreviated forms of the 17 Plenary Lectures, and two-page abstracts of the more than 450 contributed papers. Clearly, representatives of most Raman spectroscopy laboratories attended the Conference, so that the proceedings provide a valuable historical perspective of the development of the subject in the late 1980s. The flavour of the subject at this time is readily given by noting the numbers of papers contributed to the various carefully-thought-out themes of the Conference as follows: Raman Theory (6); Vibrational Analysis and Molecular Structure (24); Non-linear Raman Spectroscopy (21); SERS, Surface and Interfacial Phenomena (51); Inorganic Materials and Matrices (17); the Solid State (30); Semiconductors and Superconductors (29); Phase Transitions and Effects of Temperature and Pressure (31); Low Dimensional and Amorphous Solids (12); Resonance Raman Spectroscopy (38); Time-Resolved Raman Scattering and Transient Species (14); Biological Pigments (22); Biological Systems and Medical Applications (22); Macromolecules and Proteins (28); Lipids and Biomembranes (9); Band Shapes and Dynamics (36); Band Intensities and Molecular Conformation (11); Raman Microscopy (15); New Techniques (21). There were 21 additional papers that were received too late for classification.

On the applied side, an important current theme is the maturing of FT-Raman spectroscopy in the near-infrared region. This technique has the major advantage of the much-reduced or eliminated fluorescence backgrounds that have bedevilled earlier uses of Raman methods in industrial research laboratories. In terms of types of sample, it is clear from the above list that all types from gases to solids or, in chemical terms, from inorganic semiconductors and superconductors to biological systems, can very profitably be studied by Raman or Resonance-Raman methods. A remaining challenge is to find the sensitivity to obtain Raman spectra of adsorbed monolayers on metal surfaces other than for those, such as silver, gold and the alkali metals, where Surface-Enhanced Raman Spectroscopy (SERS) is applicable. Other interesting themes, ripe for further development, include the extension of Raman spectroscopy into the ultraviolet region, and the uses of time-resolved methods based on visible lasers to probe transient processes in gases, liquids or in photobiological systems.

The production and structure of this conference volume is also of wider interest and is to be commended. By close co-operation between the publishers and the meeting organisers, a very substantial achievement was that the complete volume was presented to those attending the meeting. In part this was made possible by asking plenary lecturers (doubtless much to their relief!) to provide only extended summaries of their contributions, and those contributing papers also to provide only extended abstracts.

In the opinion of your reviewer, too many organisers, who wish to mark the success of their conference by publishing a volume of proceedings, request both plenary and contributory speakers to produce papers of substantial length. These are often necessarily reshaped, and therefore partially redundant, forms of those that the authors are careful to publish in one or another of the well-established journals that are more widely available in libraries.

The present volume provides a substantial landmark in the still rapidly evolving research field of Raman spectroscopy. Sir C. V. Raman would have been astonished by it! It is a volume which every practitioner in the field would benefit from having on his or her bookshelves as a summary of the present state-of-the-art. However, the size, and therefore the cost, will be a deterrent to those who did not receive copies of it at a reduced price when they attended the meeting.

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