Book Reviews

Methods of Protein and Nucleic Acid Research. Volume 3: Chromatography. By Lev A. Osterman (Institute for Molecular Biology, Moscow). Springer-Verlag: New York. 1986. xii + 505 pp. $119.00. ISBN 0-387-16855-9

This third volume in the series offers chapters on theory, materials, equipment, various column modes—size-exclusion, hydrophobic, adsorption, ion-exchange, affinity—and thin-layer chromatography. The author makes a strong effort to be contemporary, with some references as late as 1985, but the orientation is basically "classical", with great (and successful) attention to chromatographic mechanisms, characteristics of sorbents, particularly commercial ones, and the operation of low-pressure systems. And while there are many examples given of recent uses of chromatography in the purification of proteins and nucleic acids, they are simply lifted from published articles without critical evaluation. Perhaps most serious is the near absence of any guide to the selection of methods. An idea of the emphasis can be formed from the allocation of space: The chapter on concepts contains 36 pages of detailed and clear description, but only 2 are devoted to macromolecules; Equipment comprises 25 pages on low-pressure chromatography, 10 on HPLC, and 4 on Pharmacia's FPLC system; Gel Filtration has 14 pages on commercial matrices, 25 on operational details of low-pressure systems, 8 on HPLC, and 4 on TLC; the section on reversed-phase HPLC, perhaps the most popular chromatographic method in current use, reserves 21 pages for small molecules, 7 for proteins, and 1 for nucleic acids; the long chapter on affinity techniques devotes 50 pages to the activation and reaction of supports (well-presented and comprehensive), 10 pages on selecting and performing the chromatography, and 35 pages of examples which, I suggest, no one will read. There are two appendices, one on protein sequenators, describing only Beckman's spinning cup, and the other on amino acid analyzers, meaning Moore and Stein ion-exchange with ninhydrin detection (pre-column methods for amino acids are mentioned under RP-HPLC).

The text is a translation from the Russian, and not a very good one. Sentences are usually intelligible, at least to one familiar with these methods, but occasionally the meaning is completely obscure. This would be somewhat more than inconvenient to novices who, given the special strengths of the book, should be the ones most able to profit from reading it. This is unfortunate, as the explanations of chromatograhic processes seem inherently very clear and well through out.

In summary, this book is successful as a introduction to chromatography in general and to methods used by researchers of proteins or nucleic acids, and as a source of data on commercial sorbents. It suffers from being several years out of date (unavoidable), infelicitously translated, and inadequate in critical evaluation and guidance.

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Advances in Chemical Physics. Volume LXII. Memory Function Approaches to Stochastic Problems in Condensed Matter. Edited by M. W. Evans (University College of North Wales) and P. Grigolini and G. Pastori Parravicini (University of Pisa). John Wiley and Sons: New York. 1985. xiv + 556 pp. $84.95. ISBN 0471-80482-7

Memory functions are used in physical chemistry to describe the time dependence of various correlation functions associated with spectroscopic information or with transport coefficients. They have been used by chemists for these purposes for more than 20 years. Recently, a group of (mainly) physicists have realized that memory functions are useful in many problems of condensed matter science. The present volume arose from that realization.

This is definitely a review; 23 authors contributed to 12 chapters. Much of the material covered here can be found in other places, but this is a compilation of a lot of material in one volume and should be useful for students.

The introductory chapter, by Grigolini, sets the stage with a careful review of the main ideas and the historical development of the subject.

The third chapter, by Grosso and Pastori Parravicini, gives a valuable summary of the properties of continued fractions in the theory of relaxation. This is material that is both very important and hard to find—courses in mathematical methods seldom mention continued fractions, which is unfortunate. The fourth chapter, by the same authors, reviews the use of memory functions in solid-state physics. Here one finds the Lanczos algorithm, recently popularized in a number of papers in chemical physics, and its relation to the recursion method, well known in solid-state physics. These two chapters are perhaps the most useful part of this volume.

Chapters 5, 6, and 7 deal with applications of the general theory and have essentially the character of research papers. (One of these is on the dynamical behavior of hydrogen-bonded liquids.) Chapters 8 and 9 contain reviews of the theory of EPR spectra and of chemical reaction rates. The remaining chapters, concerned with analogue simulations of noise, population genetics, and astrophysics, will probably be of little interest to chemists.

Overall, the quality of this volume is high. While it may not be the best place for a novice to start learning about memory functions, it should be on the bookshelf of all chemists who need to use them.

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Advances in Quantum Chemistry. Volume 18. Edited by P.-O. Lowdin (University of Florida). Academic Press: Orlando, FL. 1986. viii + 350 pp. $99.50. ISBN 0-12-034818-7

The *Advances in Quantum Chemistry* series has become a highly regarded source of review articles on topics of current interest in quantum chemistry. This latest volume maintains the high standards set by previous issues by presenting five useful and timely articles describing recent progress in active areas of research.

The first article, by I. B. Bersuker and I. Ya. Ogurtsov, presents a theoretical analysis of the Jahn–Teller effect and its influence on the electrical properties of molecules. Vibronic interactions in systems with degenerate and nearly degenerate states can cause a lowering of the molecular symmetry and, thus, influence the molecular multipole moments and polarizabilities. The authors derive expressions describing the extent of these effects and their implications for the pure rotational spectra, birefringence, and depolarized light scattering of such molecules. Some effects described by the authors remain to be thoroughly verified in the laboratory and pose a challenge for experimentalists.

The next paper, authored by J. S. Kwiatowski, T. J. Zielinski, and R. Rein, reviews the state of the art in calculating equilibrium constants for tautomeric equilibria. This subject is of considerable biological interest because minor tautomeric forms of bases, in small equilibrium concentrations, may be responsible for the occurrence of spontaneous mutations. The article describes and critically examines various approximations and models that have been used to calculate tautomeric equilibrium constants, beginning with the relatively simple case of a ground-state molecule in the vapor phase and ending with the complex case of an excited-state molecule in solution.

The dynamics of molecular crystals is the topic of an article by W. J. Briels, A. P. J. Jansen, and A. van der Avoird. This paper reviews the theoretical techniques that have been developed for calculating the frequencies and amplitudes of lattice vibrations (phonons, librons, and rotons) of such solids. After a detailed discussion of the formation of the crystal Hamiltonian from interparticle potentials, the article presents an overview of techniques for treating low-amplitude molecular motion, including the standard harmonic approximation, the perturbation theory of anharmonic corrections, and the self-consistent phonon method. Since these approximations are not applicable to molecules which undergo large-amplitude motion (e.g., strong angular oscillations), the paper describes additional techniques that are suitable for these cases. These methods include the classical dynamics technique, the Monte Carlo method, the mean field model, the time-dependent Hartree method, and the random phase approximation. The concluding sections of the article illustrate the various approximations by examining their predictions for the lattice dynamics of solid oxygen and nitrogen.

The final two articles describe related approaches to the treatment of the electron correlation problem. A paper by M. R. Hoffman and H. F. Schaeffer, III, gives a derivation of the full coupled-cluster model including single, double, and triple excitation operators. It presents the resulting coupled-cluster equations diagramatically and algebraically and discusses strategies to render the technique computationally feasible. An article by S. Kucharski and R. J. Bartlett describes how various coupled-cluster methods are related to perturbation theory. It presents an iterative scheme for obtaining many-body perturbation theory diagrams to fifth order from the more easily generated coupled-cluster diagrams. The paper also discusses computational aspects of the proposed perturbative treatment.

This volume contains much useful information and many interesting insights. It will prove valuable to individuals who are actively performing research in the areas covered, those who wish to enter these fields, and those who simply want to keep in touch with ongoing developments in modern quantum chemistry.

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