

regions, respectively. The last three chapters cover some of the applications of optoacoustic spectroscopy. Vapor phase applications are discussed first for the infrared region, Chapter 6 (Claspy) and the visible and ultraviolet regions, Chapter 7 (Robin). Finally, the applications to solid state samples is covered in Chapter 8 (Rosenwaig). References at the end of each chapter include citations through 1976.

Better editing of the individual chapter to remove some of the repetitious discussions concerning the basic mechanisms of signal generation and transduction as well as the design of the detector itself would have created space for some of the other topics which were not as well covered. For example, the text does not include a rigorous discussion of quantitative analytical data treatment. Although this omission may be due to the youth of the field or to the backgrounds of the authors, most chemists would consider it serious. Further, at no single point in the text is there a general discussion of the relative merits of optoacoustic spectroscopy in comparison with other more conventional forms of spectroscopy.

Any recommendations for the usefulness of this book has to be made weighing the strengths and weaknesses of the text. Chemists looking for an introduction to this newer spectroscopy may be disappointed in this text; however, chemists faced with applying this method to a specific problem would be well advised to include the appropriate chapters of this book in their reading lists.

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#### Statistical Treatment of Experimental Data

*J. R. Green, and D. Margerison*, University of Liverpool. Elsevier Scientific Publishing Co., Amsterdam, 1977. Figs. & tables. 15.5 × 23 cm. x + 382 pp. \$34.95.

This book presents a rigorous treatment of statistical methods which may be employed to handle experimental data and the extent to which useful conclusions can be drawn from the data. The coverage is extensive and highly mathematical. Numerous examples of the applications of statistical analysis to typical experimental data sets are provided including a liberal representation from several areas of chemistry.

The approach adopted in this book is far beyond that required for undergraduate courses in the physical sciences, since selected chapters in most existing textbooks treat this topic adequately. Instructors in physical chemistry laboratory courses would find the text a useful addition to their personal bookshelf, and it is strongly recommended as a reference source for the library.

For the researcher who is involved in handling large quantities of data and for those whose primary interest is the critical compilation and evaluation of data, this book provides a well-balanced and thorough treatment of various approaches used for analyzing data.

The authors have stressed the need for assuming some probability model on which

to base any statistical analysis of data, and three chapters are devoted to a detailed discussion of probability theory, including probability distributions such as the binomial, Poisson, normal, and exponential distribution.

For those working with limited sets of experimental points, there are two chapters dealing with the theory and practice of the estimation of the unknown parameters of density or distribution functions and includes a treatment of least squares, method of moments, and the Bayesian method. All the methods are well illustrated with examples. A detailed explanation is provided on the computation of a confidence interval for the unknown parameters.

Hypothesis testing is the subject of a separate chapter and deals with formal procedures for testing hypotheses. Subsequent chapters apply these concepts with well illustrated examples to tests on means, variances, and goodness of fit. The tests are restricted mainly to the normal distribution. The goodness of fit tests address the question as to the validity of whether the selected probability distribution or particular form of a probability distribution is, in fact, appropriate by examining several procedures for testing how well the data fits the probability distribution in question.

For those involved in teaching chemistry laboratories for advanced classes chapters 12-15 should be of particular use in improving one's general background. These chapters discuss the situations where the straight line or polynomial is constrained to pass through

the origin or some other fixed point and includes a detailed presentation of least squares analyses, the need for weighting factors, and demonstrates concrete examples of confidence intervals, inverse interpolation, hypotheses testing, and goodness of fit models.

Also included in this book are discussions of rounding-off errors and the choice of the number of significant figures.

The text has been produced using a photo-offset method, but it is well organized, clearly presented, and free from any major errors. It is certainly too expensive for student purchase, but it is not unreasonably priced for acquisition by libraries, and by researchers and teachers who are directly involved with the analysis of data.

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#### Classical Kinetic Theory of Fluids

*P. Resibois, and M. De Leener* Free University-Brussels. John Wiley & Sons, New York, 1977. Figs. 15.5 × 23.5 cm. xv + 412 pp. \$29.50.

The stated goal of this work is to present a coherent and self contained introduction to  
(Continued on page A186)

## book reviews

the techniques of nonequilibrium statistical mechanics as applied to the treatment of simple (that is, no internal molecular structure) classical fluids. In my opinion, the authors achieve admirable success in attaining this goal. The treatment presented combines a scholarly, authoritative approach to the subject with a writing style that is clear, readable, and sometimes even entertaining.

The book is divided into four main sections, each of which discusses a specific aspect of the overall theory. Part A deals with the stochastic approach, using as an example the classical theory of Brownian motion. A particularly appealing feature of this section is an understandable introductory chapter on necessary concepts from probability theory. Part B describes the classical kinetic theory approach. It proceeds from development of the Boltzmann equation to a discussion of approximate (linearized) solutions which permit the calculation of dilute gas transport coefficients. A closing chapter of the section describes extension of kinetic theory ideas to a dense hard-sphere fluid. Part C deals with the modern, purely microscopic approach and proceeds via the Liouville equation to develop the generalized kinetic equation governing nonequilibrium processes. A chapter on applications of the general theory demonstrates that in appropriate limits, results of the generalized treatment reduce to those obtained from the stochastic and kinetic theory approaches. A closing chapter of the section describes difficulties associated with extending the Boltzmann equation to higher densities. Part D describes correlation function formalism and demonstrates how it can be used to obtain a unified treatment of macroscopic response to external perturbations. A final chapter deals with the calculations of time-dependent correlation functions and includes a discussion of results from recent computer experiments.

By adopting a quadripartite treatment of the subject and by working from the more specific to the more general with frequent backward references, the authors achieve as an end result a nicely interwoven picture of available approaches to the theory of nonequilibrium processes. Inevitably, however, this picture comes at the sacrifice of an element of logical organization and unidirectional flow. As a result, the work is rendered less useful as a source for quick reference on a specific topic.

It should be noted that the level of mathematics used throughout the presentation would probably be considered high by most practicing chemists. Thus, although derivations are presented with clarity, a complete comprehension of them often requires competence in topics (for example, Laplace transforms, Fourier analysis, complex variables, operator algebra, etc.) often treated lightly (if at all) in a chemistry curriculum. On the other hand, it should be noted also that in many instances, the clarity of the text is such that the essence and importance of a result can be understood, even though the detailed route to it may be obscure.

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### Dynamics of Molecular Collisions, Parts A & B

W. H. Miller, Editor. Plenum Press, New York and London, 1976. xiii + 317 pp. Figs. & tables. 17 × 25.5 cm. \$39.40. (Part A). xv + 380 pp. Figs. & tables. 17 × 25.5 cm. \$39.50. (Part B).

A recognizable goal of the science of chemistry is the acquisition of better understanding of the observed behavior of matter in terms of its ultimate structure and the interactions between its component parts. The success of acquiring insight into the structural nature of matter, at least at the atomic and molecular level of interest to most chemists, has far outweighed the success of understanding the details of atomic and molecular interactions. The gap, however, is narrowing as a result of intensified activity in the study of those phenomena. Reports on these activities have so proliferated that considerable effort is necessary to keep abreast of the field. Fortunately we are blessed from time to time with comprehensive, in depth reviews of portions of the field. These provide helpful summaries of the state of the art and offer a convenient means of introducing the subject to newcomers.

The latest such review, "Dynamics of Molecular Collisions," edited by William H. Miller, comprises the first two volumes of a contemporary treatise: Modern Theoretical Chemistry. The purpose of the editor and contributing authors is to survey the many advances in theories of molecular impact phenomena which have been stimulated by dramatic advances in experimental methods of observing effects of these phenomena. The first volume (Part A) deals mainly with quantum dynamics of inelastic and reactive collisions. Its chapters reiterate the familiar story that although those dynamical behaviors of matter which correctly invoke the uncertainty principle via solutions of the Schrodinger equation are the ones which will correctly predict the observed behavior of real systems, the exact solutions for most systems of chemical interest remain elusive. The reader, however, is updated on the many methods devised to extract approximate solutions. As well as chapters dealing with general molecular scattering theory, the volume includes chapters on special topics including optical models, vibrational energy transfer, nonradiative processes, and scattering by surfaces.

The second volume (Part B) is concerned mainly with classical and semiclassical treatments of molecular dynamics. It contains chapters on trajectory calculations, nonadiabatic collision processes, statistical approximations, and unimolecular reaction kinetics.

Since the contributing authors are highly qualified experts in the fields of their reports, the quality of the work is outstanding. The work is suitable for use by graduate students with a good mastery of both classical and quantum mechanical principles including theories of scattering. Either one or both of the volumes could serve well as textbooks in an advanced course on molecular dynamics. The student will find exposure to at least some of the materials in the more than 1100 footnoted references. The work includes a complete author index and a fair subject index.

In works of this nature, each chapter is a separate entity with its own expository

quality and style. Each reader is sure to find something that is particularly impressive to him individually. The reviewer, for example, found two of the thirteen chapters especially pleasant reading. In his report on the effects of potential energy surfaces on molecular collisions, P. J. Kuntz points out explicitly his intention to emphasize the general relationships between the geometric features of potential energy surfaces and the course of molecular dynamics in favor of the less intuitively obvious connection between the dynamics and the potential, when the latter is given in tabular numerical form. Chemists who are not already accomplished experts in the subject will probably comprehend the implications of these relationships more quickly by Kuntz's approach, especially with the aid of his excellent trajectory diagrams, than by a study of *ab initio* potential calculations. At any rate it might be wise for the beginner to read this chapter early in the study.

The final chapter, "Thermodynamic Approach to Collision Processes" by R. D. Levine and R. B. Bernstein is probably the most exciting and intellectually stimulating report in the entire work. These authors explain the efforts underway to "bridge the gap between thermodynamic and kinetic points of view." The report is valuable not only for its substance which one might assume stems from a novel approach to the problem, but also for an important lesson that all scientists might well learn. The basis of the thermodynamic approach is not new but was anticipated by Gibbs and others years ago. The birth of quantum mechanics, however, diverted attention from thermodynamics to the point that these ideas were not pursued until recently, and the fruits of this approach are only now beginning to appear. Surely we would be wise not to abandon established methods of investigation while they still have useful momentum.

I recommend the entire work to all those who are interested in collision dynamics and the final chapter (Chap. 7, Part B) to all chemists and students of chemistry.

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### Magnetic Properties of Transition Metal Compounds

Richard L. Carlin and A. J. Van Duyneveldt. Springer-Verlag, New York, 1977. Figs. & tables. 17 × 24.5 cm. xv + 264 pp. \$18.80.

According to the authors R. L. Carlin and A. J. Van Duyneveldt, the major purpose of the book "Magnetic Properties of Transition Metal Compounds" is to acquaint chemists with the recent works of physicists. As a result this book does not focus on such chemically-oriented topics as Guoy and Faraday methods for obtaining magnetic susceptibility measurements or how one can distinguish a square planar nickel(II) complex from a tetrahedral nickel(II) complex by magnetic measurements or even on simple paramagnetic metal complexes at high temperatures.