

final hard copy. This ability to easily combine standard plots with drawings is unique among programs of this type and offers additional flexibility not found in most plotting-only programs.

The program CoDraw provides the user with the ability to draw lines, circles, rectangles, arrows, Bézier lines, and irregularly shaped figures. CoDraw can also incorporate superscripts, subscripts, and Greek characters easily into figures, but the formation of molecular structures is quite laborious (the publisher recommends a dedicated software package designed expressly for this purpose). One annoying omission in the program is the inability to make solid-filled circles, certainly a commonly used figure. As in CoPlot, the user is allowed to choose from a wide variety of formats when exporting the finished design—a definite advantage over other drawing programs.

As mentioned earlier, the CoPlot program has many features that make it attractive for use by scientists. However, we noticed some limitations in data handling that make it difficult to use with multiple data

sets. Each graph can only display nine data sets at a time from the internal spreadsheet. We found this to be a bothersome restriction, as we often wanted to plot many more than nine data sets at a time—for instance, a stacked plot of two groups of seven spectra showing changes with temperature. There are also constraints on the total number of graphs and comments that can be included in a figure, although the annotation restrictions can be overcome if the figure is sent through CoDraw before the hardcopy is produced.

All in all, CoPlot, CoDraw, and CoStat perform as described by CoHort Software. All three packages contain features that make them useful for scientific applications, but there are some limitations to CoPlot that may make it ill-suited for complicated projects. We feel that if one wants a simple, well-integrated and low-priced package, then this package is a good choice.

Douglas A. Cates, V. J. P. Srivatsavoy, and Herbert L. Strauss,  
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## Book Reviews\*

**Introduction to the Thermodynamics of Solids.** By J. L. Ericksen (formerly Department of Aerospace Engineering and Mechanics, University of Minnesota). Chapman and Hall: London and New York. 1991. xii + 204 pp. \$49.95. ISBN 0-412-39840-0.

This textbook is the first volume of the series *Applied Mathematics and Mathematical Computation*, which includes texts and monographs at graduate and research level. The series editors are R. J. Knops and K. W. Morton.

The book is based on a course offered at the University of Minnesota to seniors and beginning graduate students from various engineering and scientific departments. Although it may be of interest to a variety of chemists and other scientists, it is likely to be of greatest value to those working in the fields of mechanical and aerospace engineering. Readers are assumed to have a mastery of classical thermodynamics, statics, deformations of solid bodies, and calculus. The author has set out to cover considerable ground in only about 200 pages, which has led to some deficiencies in explanation. The book is carefully written, but it would be improved if each chapter began with a summarizing paragraph.

The book deals with aspects related to power and energy in mechanical engineering problems and places little or no emphasis on chemical aspects, such as solid solutions and phase equilibria, which have been covered by a book entitled *Thermodynamics of Solids*, 2nd ed., by R. A. Swalin, published by John Wiley and Sons: New York, 1972.

Chapter 1, Generalities, explains the first and second laws of thermodynamics and the concepts of thermal and mechanical thermodynamic equilibrium and ballistic free energy.

Chapter 2, Constitutive Theory of Heat Transfer for Bars and Plates, introduces the thermodynamics of rigid bars through the Clausius–Duhem and Clausius–Planck inequalities. This chapter develops the basic criteria for equilibrium in the absence of phase transition and a theory of heat transfer (1) for a rigid mechanically-isolated bar, (2) for a thermoelastic bar, and (3) for shearing of plates. Finally, some experimental approaches are outlined to enable the behavior of the above systems to be characterized thermodynamically. Unfortunately, the parentheses notation employed in this chapter is somewhat confusing. For example, a multiplication operator should be included after  $\theta_0$  in equation 2.1.21.

Chapter 3, Equilibrium Theory of Bars, considers two situations; bars subjected to dead loads and bars in hard devices. The chapter discusses stability in solid bars and problems associated with metastable configurations and finally introduces the equal area rule or the Maxwell line. The material is clearly presented.

The first section of Chapter 4, Equilibrium Theory of Plates, discusses Martensite, Austenite and Martensitic transformations that are related to the crystal symmetry of the material. The second section considers bifurcation diagrams, which provide a picture of the response of a system when a control variable is changed. The material is attractively presented, but the application of the Martensitic transformation is not well explained.

Chapter 5, Balloon Problems, considers spherical balloons made of a homogeneous, isotropic, incompressible material to which rubber closely approximates and applies the concepts developed in Chapter 3. Inci-

dentally, equation 5.1.5 is lacking the division operator, i.e.  $r^3/R^3$ .

Chapter 6, Biaxial Stretch in Rubber Sheets, considers the stability associated with biaxial stretching of a thin flat sheet of rubber at constant temperature. This chapter first deals with the idealized problem and then introduces the Treloar instability. This chapter would be more convincing if the application of the Martensitic transformation, introduced in Chapter 4, were better explained.

Chapter 7, Moving Discontinuities, consists of four sections: shock waves in bars, breaking bars, and two peeling problems. This chapter provides convincing theoretical background for the dynamics of failure of solids and of adhesion of one material to another.

Chapter 8, Mixture Theory, considers the thermodynamics of multi-component systems, including such materials as  $\alpha$  or  $\beta$  brass (containing copper and zinc) and wood containing various proportions of sorbed water which produces a change in volume. The treatment presented can apply to quite complex systems for which the phase diagrams and, indeed, the chemical nature of the solid materials need not to be known. Chemists who are more familiar with treatments based on phase equilibria may be stimulated by this difference of approach.

In Chapter 9, Equilibrium of Liquid Crystals and Rods, the first section, liquid crystals energies, recognizes that nematic liquid crystals, such as those in display devices, encounter equilibrium situations that resemble those in solids. The second section considers the orientation of liquid crystals by fields and walls. The third section considers the theoretical background to the measurement of mechanical moduli of liquid crystals. The behavior under strong fields may be explained by Fréedericsz transitions. The fourth and last section considers elastica theory, introduced by Euler to explain the behavior of straight, long, thin bodies when compressed along the major axis. The necessary elementary theory is well-developed in this chapter.

Chapter 10, Reconsideration of the Generalities, is the final chapter. As its name suggests, this chapter reconsiders the thermodynamic background presented in Chapter 1 in the light of the material presented in the rest of the book. Chemists to whom the material in the rest of the book is rather unfamiliar will instantly recognize much of the material in this chapter and may wish to read Chapters 1 and 10 first before embarking on a study of the rest of the book. Chapter 10 is eminently readable.

The book lists 72 references placed between Chapter 10 and the Index. The references have been judiciously chosen to be particularly useful and to range from the very elementary to the rather sophisticated. The references include textbooks, monographs, and reviews to seminal research papers. The Index is very short, but it is comprehensive enough to be useful. The book is recommended reading for scientists interested in the mechanics of solids.

David J. W. Grant, Sarma P. Duddu, and Devalina Law,  
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**Introduction to Stereochemistry & Conformational Analysis.** By Eusebio Juaristi (Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Mexico). John Wiley & Sons, Inc.: New York. 1991. xv + 331 pp. ISBN 0-471-54411-6.

This book is, as the name states, an "Introduction" and displays some of the advantages and disadvantages associated with any "Introduction". Thus, as the author notes, some areas may be covered lightly or even

\*Unsigned book reviews are by the Book Review Editor.

excluded (e.g., application of oxygen-17 NMR to determination of molecular geometry; stereochemistry of cyclohexadienes; transannular effects in medium-sized rings). Unfortunately, a brief topic index (8 pages) makes it difficult to discover if a specific item is included and may even be misleading; for example, there is no index entry for "disulfide", although there are examples of disulfide stereochemistry in the text (p 282), and the addition of  $\text{BD}_3$  to an alkene is presented on p 51, but there is no reference to  $\text{BD}_3$  (or English equivalent) in the index. The absence of any problems surprised me (especially in light of my student's responses to the problems in *Introduction to Stereochemistry*, K. Mislow; W. A. Benjamin, 1965). There are other minor flaws (e.g., inconsistent representation of "bonds behind the plane of the paper"), but they should not present a significant obstacle to the reader. On the more positive side, I welcomed Chapter 3 ("Stereochemical and Conformational Descriptors") and found the general selection of topics covered to be interesting and the depth of coverage adequate. The sequence of topics was reasonable although I would have discussed "The Conformational Analysis of Acyclic and Cycloalkanes" (Chapter 14, p 237) earlier. I was particularly pleased at the extensive use of structures and reaction schemes.

There is a shortage of textbooks of organic stereochemistry and this book helps to meet this need.

A. L. Ternay, Jr., University of Texas at Arlington

**Maximum Entropy in Action. A Collection of Expository Essays.** Edited by Brian Buck and Vincent A. Macaulay (University of Oxford). Clarendon Press: Oxford, 1991. xxvii + 220 pp. \$65.00 (cloth) or \$35.00 (paperback). ISBN 0-19-853941-X.

Following eight pages of the editors' introduction, this book consists of eight chapters, each  $27 \pm 10$  pages in length. Use of the  $\pm$  symbol here is appropriate since, as the editors' concede, "maximum entropy" really deals with "maximum uncertainty" or "principle of greatest multiplicity" rather than thermodynamical entropy. The editors have long been interested in "going from incomplete and noisy data to a description of the underlying physical system" and present the principle of maximum entropy as a way to help this situation. The editors arranged a series of interdisciplinary research seminars at Oxford and have gathered the published versions of the lectures in this book. These lectures were presented at a relatively sophisticated level, so the reader may not fully appreciate the presentations unless he or she has some familiarity with topics such as probability calculus, deconvolution, Bayes' theorem, and symbolic logic. In recent years a number of books, easily understood by those with only modest mathematical skills, have been published on chaos. This book on MaxEnt, as it is fashionably called, is directed to a more select group of specialists.

In the introduction, the editors present a clear overview of MaxEnt, which stems from the work of Claude Shannon in communication technology. He utilized probability theory to present the formula for determining the number of yes/no questions that must be asked to determine which of  $N$  propositions is true:  $S = -k \sum_{n=1}^N p_n \ln p_n$ . Here  $k$  is a suitably selected constant, and each  $p_n$  is the probability that a particular proposition  $n$  is the correct one. The form of the above equation is of course identical in form to Planck's expression for thermodynamical entropy. E. T. Jaynes' determined the underlying connection between the two, and this led to the development of maximizing uncertainty (MaxEnt).

The book describes in two chapters the rationale of the MaxEnt method and then three chapters are devoted to applications. Two additional chapters deal with the interpretation of thermodynamic entropy, and the last one discusses the X-ray crystallographic phase problem. Chapter 1 (Of maps and monkeys: an introduction to the maximum entropy method by G. J. Daniell) effectively uses seven figures to give an overview of how MaxEnt is applicable to data handling. The philosophy of data processing is logically presented, and the utility of MaxEnt is clarified with an instructive example. Chapter 2 (Fundamentals of MaxEnt in data analysis by J. Skilling) according to the editors is not an easy chapter. This is true. Probability calculus leads to image reconstruction, the probability of an image, and the deconvolution of Poisson data. Nonetheless, the sophisticated arguments presented here provide the rigorous basis for MaxEnt. Chapter 3 (Maximum entropy and nuclear resonance by P. J. Hore) describes how the MaxEnt method can be used as an alternative to Fourier transformation in NMR. FT methods have the disadvantage that any defects in the data are transferred into the frequency domain. The MaxEnt approach proceeds from the frequency domain to the time domain. Here, from a large number of *guessed* trial spectra, many may be rejected for bearing no resemblance to the experimental free induction decay. This chapter shows how the MaxEnt method may be used to process NMR data and indicates where this might be profitable. Somewhat surprisingly, however, the author concludes that FT methods may in fact be superior since NMR data are not

grossly distorted and are well suited to conventional processing methods. Chapter 4 (Enhanced information recovery in spectroscopy using the maximum entropy method by S. Daives, K. J. Packer, A. Baruya, and A. I. Grant) deals with applications to Raman as well as NMR spectroscopy. In contrast with the previous chapter, it makes a strong case for the utilization of MaxEnt methods, especially for Raman spectroscopy. A total of 24 figures primarily showing reconstructed spectra are very impressive. The reader cannot readily expect to run his PC and put MaxEnt into operation, but assistance from the authors (all at BP Research Centre) or S. Gull and J. Skilling, co-founders of Maximum Entropy Data Consulting Ltd., would probably make its utilization feasible. Chapter 5 (Maximum entropy and plasma physics by G. A. Cottrell) may prove to be of less interest to chemists although it also deals with spectroscopy deconvolution and FT spectroscopy. Some attractive two-dimensional spectral reconstructions are shown among the 16 figures. Chapter 6 (Macroirreversibility and microreversibility reconciled: the second law by A. J. M. Garrett) is a "crash course in Bayesian techniques" and assumes a "certain mathematical sophistication" of the reader. It describes "how the correspondence difficulties of the second law of thermodynamic disappear when the methods of statistical physics are recognized as instances of reasoning from incomplete information." (The editors described this chapter very well.) In Chapter 7 (Some misconceptions about entropy by S. F. Gull), the shortest, the author amplifies some of the arguments of the previous chapter. Among other topics, Gibbs versus Boltzmann entropies, Brownian motion, and time asymmetry in physics are dealt with. Chapter 8 (The X-ray crystallographic phase problem by G. Bricogne) treats the demanding inverse problem associated with the analysis of X-ray diffraction patterns. It is shown that the MaxEnt method is essentially equivalent to the often used saddlepoint approximation. The author states, true to the style of much of the text, that the "reader may share the writer's relief at having replaced the invocation of an all-embracing epistemological argument by the certainty of a purely analytical derivation."

In summary, this is a significant text which is not easy reading but provides valuable material for those of us involved with data analysis. The applications of MaxEnt methods to spectroscopic analysis are especially interesting.

Jaen Laane, Texas A&M University

**Metal-Surface Reaction Energetics. Theory and Application to Heterogeneous Catalysis, Chemisorption, and Surface Diffusion.** Edited by Evgeny Shustorovich (Eastman Kodak Co.). VCH Publishers Inc.: New York, Weinheim, and Cambridge, 1991. vii + 232 pp. \$75.00. ISBN 3-527-27938-5.

The title is esoteric. The subtitle is specialized. This is an edited book containing five chapters written by eight authors. It is not a "book" to read from beginning to end, but as I kept perusing this handsomely printed and well-edited volume, I learned so much that I wish to convey my message to a small but very successful group of chemists and chemical engineers in heterogeneous catalysis: there is a lot to learn in this book, not so much in theory but in the facts that the theorists who wrote the book are trying to explain today with the faint hope that tomorrow they will actually predict new chemistry in as yet unknown catalytic cycles.

So what do we read in this book? Question: "Why does  $\text{H}_2$  dissociate without a barrier on a nickel surface but with a barrier on a copper surface" (p 40)? A possible answer is from "pure orbital symmetry arguments, in a similar fashion as symmetry arguments are used to qualitatively describe chemical reactions between organic molecules using the Woodward-Hoffmann rules" (p 46).

A recurrent theme in the book is the Bond-Order-Conservation (BOC) phenomenological theory developed in the past ten years by the editor of the book. This theory starts with the concept of bond order in the sense of shared electron pairs following G. N. Lewis, Linus Pauling, and Harold Johnston. Recent developments have been very successful in obtaining, in a deceptively simple manner, the energy of bonds at metal surfaces as well as the activation barrier for adsorption, desorption, surface reaction, and surface diffusion, all on metal surfaces. The BOC method is accessible to all, and examples of its application permeate the book. Many known results from surface science at metal surfaces can be "predicted" post facto by BOC calculations. In turn, new results can be obtained in poorly charted domains, e.g., adsorbate-adsorbate interactions at metal surfaces (p 140). Thus, the BOC approach combined with a Monte-Carlo simulation shows that adsorbate-adsorbate interactions account for a puzzling phenomenon of adsorption assisted desorption at metal surfaces (p 220).

At the frontier of surface science, a small group of pioneers are studying the state-to-state dynamics of processes at single-crystal metal surfaces. It is comforting to know that the rules formulated 20 years ago by John Polanyi for gas-phase reactions are now substantiated for surface

processes as well (p 186): these rules tell us when, in an elementary step, translational energy aids reaction and products are vibrationally excited, and when vibrational energy aids reaction and products are translationally excited.

In summary, this collection of personal accounts of progress in the theory of surface processes at metal surfaces can be a revelation to the experimental scientist of the wealth of facts that are currently being attacked on a broad front, from the BOC approach to quantum dynamics of gas-surface processes. There is some jargon in this book, but a minimum of it, most probably as a result of stern editing. As usual, a better index would facilitate random reading, the only way to appreciate a book of this kind. Indeed, if it is true that appetite is aroused by eating, curiosity grows with grazing this very rich fare of surface phenomena. This book is a great anthology of current surface chemical physics.

Michel Boudart, *Stanford University*

**Transition Metal Nuclear Magnetic Resonance. Studies in Inorganic Chemistry 13.** Edited by P. S. Pregosin (Swiss Federal Institute of Technology). Elsevier: Amsterdam and New York. 1991. xi + 351 pp. \$188.50. ISBN 0-444-88176-X.

Transition metal NMR has experienced an exceptional growth in recent years. Modern instrumentation which allows direct detection of many metal nuclei is now widely available. Indirect methods still, however, offer the best advantages for low-abundance or low-sensitivity nuclei. INDOR, which still provides an efficient and convenient method for determining approximate chemical shifts, has largely been supplanted by newer pulse methods such as INEPT and reverse or inverse detection. This has allowed a gain for  $^{183}\text{W}$  of 2830 in sensitivity or a time advantage of nearly  $10^7$ . For example,  $^{183}\text{W}$  NMR on a 1-mg sample can be obtained in 1 h with indirect  $^1\text{H}$  detection or 5 h with 2D ( $^{183}\text{W}, ^{31}\text{P}$ )- $^1\text{H}$ . Only recently have spectrometers become available that have the stability and computer power to carry out these experiments. In effect, this book surveys the practical application of these methods, as well as providing a review of transition metal NMR.

The text is organized by group number in the periodic table; however, there is no chapter specifically devoted to the practical aspects of obtaining spectra. This information is scattered within the chapters by different authors, as it pertains to specific nuclei. The reader might be well served by first reviewing portions of the chapters by Mann (pp 178–190), Benn (pp 105–114), and Brevard (pp 82–88) to become acquainted with the new techniques, their limitations, and the jargon associated with them. Some of the most promising inverse detection techniques, e.g., ( $^{31}\text{P}, ^\text{A}\text{M}$ )- $^1\text{H}$ , may still be available only to specialists who have probes capable of simultaneously being tuned for two other nuclei, decoupling protons, and locking on deuterium.

Since the effects of quadrupole moments and chemical shift anisotropy can sometimes make a solid-state MAS NMR experiment the method of choice, it is fortunate that both solution and solid state results are included in the reviews. The editor is also to be congratulated on the liberal inclusion of spectra, as opposed to providing only tabulations of shifts. In this regard, several of the chapters nicely illustrate the breadth of chemistry that can be gleaned from NMR studies; Pregosin's section on  $^{195}\text{Pt}$  is particularly informative.

As the book was directly reproduced from manuscripts, there is considerable variability in quality of presentation and line spacing within the chapters. On the whole, the quality is fairly high and the faster production of the book was a reasonable compromise between aesthetics and keeping the contents up to date. A book of this size cannot be comprehensive; nevertheless, it provides adequate reference to reviews of the literature. It provides an excellent survey of the field up to 1990. It will certainly be of interest to those planning to make use of transition metal NMR.

J. W. Faller, *Yale University*

**Topics in Fluorescence Spectroscopy. Volume 1. Techniques.** Edited by Joseph R. Lakowicz (University of Baltimore Medical School). Plenum Press: New York and London. 1991. xiii + 453 pp. \$79.50. ISBN 0-306-43874-7.

This first volume in a set of three is devoted to a description of a number of modern techniques based on fluorescence emission. In the first

four chapters the authors describe several aspects of time-domain fluorescence decay measurements with a strong emphasis on sources and the principles and strategies of detection. A small chapter is dedicated to the emerging use of synchrotron radiation as a source of excitation in these experiments. The chapters are written by experts in the field and are thorough and informative. The style is clearly intended to provide useful information for the experimentalist and covers a number of practical issues from instrument design to principles of data analysis. The interpretation of data is touched on, but not elaborated upon in detail. Presumably Volumes 2 and 3 will dwell more on issues of applications and interpretations. Chapter five, written in part by the editor, establishes the principles and usefulness of frequency-domain fluorescence decay measurements. The chapter is quite complete in its presentation of the theory, the instrumentation, and the applications of the technique.

The first five chapters of Volume 1 contain excellent descriptions of the current approaches to measurements of fluorescence emission lifetimes and provide the non-expert with a clear picture of the state of the art in experimentation and analysis. In particular, they provide a very nice comparison between the time-domain and the frequency-domain approaches and illustrate the advantages and limitations of the two complementary techniques. Review of applications to specific chemical or biological systems is reserved for later volumes. Newcomers to the field could consult Chapters 1–5 for technical details on sources and detection schemes as well as potential pitfalls of the measurements. Experts in the field will probably be familiar with most of the information presented, but may find useful details. These first five chapters have excellent bibliographies and will be useful reference sources for anyone interested in fluorescence lifetime measurements.

Chapters 6–8 diverge from the thrust of the first five chapters by describing fluorescence correlation spectroscopy, fluorescence microscopy, and flow cytometry.

The sixth chapter is a complete overview of the field of fluorescence correlation spectroscopy and should be of interest to anyone interested in modern fluorescence techniques. The principles of this relatively unexplored approach to measuring diffusion, chemical kinetics, and aggregation are explained in detail with a good description of the theory and recent examples of application. The bibliography is current and complete.

Chapter seven is focused almost entirely on microscope optics and is basic and descriptive. Chapter eight is likewise descriptive in nature but does provide the basic information on the principles and the scope of the flow cytometry measurements. These last two chapters are quite disappointing. They are too general to be useful for the experimentalist and yet too selective in the scope of the description to provide insight into the usefulness or purpose of the techniques. Better reviews of these approaches exist elsewhere. Nevertheless, both chapters have extensive and current bibliographies.

Overall, Volume 1 appears to be directed primarily at the chemist or biologist interested in understanding or getting involved in using fluorescence lifetime techniques. It serves this purpose very well but could have done so with the first five chapters only. It will be interesting to see whether Volumes 2 and 3 provide current reviews of the scientific applications of these techniques. Chapter 6 is a novel, interesting, and useful inclusion, but Chapters 7 and 8 should not be the reason to acquire the volume.

Nils O. Petersen, *The University of Western Ontario*

**Particles on Surfaces. Volume 3. Detection, Adhesion, and Removal.** Edited by K. L. Mittal (IBM US Technical Education). Plenum Press: New York and London. 1991. viii + 328 pp. \$89.50. ISBN 0-306-44180-2.

This book contains selected papers from the Third Symposium on Particles on Surfaces: Detection, Adhesion, and Removal held as a part of the 21st Annual Meeting of the Fine Particle Society in San Diego, CA, August 21–25, 1990. It contains 24 chapters, in typescript form, organized under the following headings: Part I. Particle-Surface Interactions, Adhesion and General Papers; Part II. Particle Detection, Identification, Analysis and Characterization; and Part III. Particle Reduction and Removal. There is a section at the end titled "About the Contributors", which gives brief biographies of the authors of the chapters. A subject index completes the book.