Additions and Corrections

Light-Scattering Studies on the Thermally Induced Crystallization Transition of β-Cyclodextrin [*J. Am. Chem. Soc.* **1995**, *117*, 9314−9322]. YANNIS GEORGALIS,* JENS SCHÜLER, PATRICK UMBACH, AND WOLFRAM SAENGER

Due to a mistake in a program performing the linear regression to the ln K versus $1/T$ data we have obtained values for the free entropy, $\Delta S = 0.405 \pm 0.016$ kJ mol^{-1} K^{-1}, of nucleation from intercepts that were twice divided by a factor of 10^3 while converting J to kJ. We have therefore erroneously concluded that the product $-T_m\Delta S$ is negligible compared to ΔH.

The value of the free energy of nucleation is overestimated by a factor of 1.8; it should read $\Delta G = -227$ kJ/mol. Figure 4 of our paper should then be modified accordingly, i.e., the y-axis should extend from −317 to 317 rather than −160 to 160. Also in error by the same factor is the $\Delta\Delta G$ value that typifies the crystallization−dissolution process. It should read $\Delta\Delta G = 52$ kJ mol^{-1}. All other conclusions remain unaffected.

JA965402E

Book Reviews

One-Dimensional Metals Physics and Materials Science. By Siegmar Roth (Max-Planck Institut für Festkörperforschung). VCH: Weinheim. 1995. xii + 247 pp. $95.00. ISBN 3-527-26875-8.

The book is the result of a series of lectures given by the author at the University of Karlsruhe. It consists of 10 chapters, which are (1) Introduction, a general introduction; (2) One-Dimensional Substances, an overview of one-dimensional solids; (3) One-Dimensional Solid State Physics, a good introduction to reciprocal space and solid state physics; (4) Electron-Phonon Coupling, Peierls Transition, the unusual effects of low-dimensionality; (5) Conducting Polymers: Solitons and Polarons, mostly a discussion of polyacetylene; (6) Conducting Polymers: Conductivity, a very simple introduction to electron transport; (7) Superconductivity, a very good introduction to the subject (on a pedantic note, I would not have written a subtitle One-Dimensional Organic Superconductors, simply because superconductivity cannot be supported in one-dimension); (8) Charge Density Waves, a more in-depth examination of the Peierls transition; (9) Molecular Electronics, essentially potential applications; and (10) Applications, genuine applications. Though the book is directed to a physics graduate student audience, it should be understandable by physical or physical organic chemistry students. It includes references as recent as 1994.

The field of low-dimensional materials is replete with edited books and proceedings of conferences but a *good*, one-volume, single-author book does not exist. While *One-Dimensional Metals Physics and Materials Science* comes close, it, unfortunately, does not fill the vacuum. It is not intended to be an in-depth study, brimming over with references. The book could be recommended as a text for a "special topics" course in chemistry or physics, provided it is edited properly (see below).

This book is alive with cartoons which inject well-intentioned humor and make the reading of the book entertaining. Dr. Roth is notorious for his scholarship which is reflected in a number of knowledge nuggets, normally absent in monographs of this sort.

The chapters on solid state physics (Chapters 3 and 4) are the best. It is clear that the subject is familiar and dear to the author. On the other hand, the chapters which include chemistry and broader concepts were not developed to the same extent. Chapter 2 has some serious errors in concept. For example, in an attempt to explain the Jahn−Teller distortion with a figure, there are two gross errors: (1) before the alleged distortion, there is a violation of Hund's second rule (two electrons in degenerate, half-filled orbitals are shown with *opposite* spins), and (2) after the distortion, the depiction is of two electrons *in two half-filled, degenerate orbitals*!

One gets the impression that this book was rushed to print. The book is full of typographical errors, spelling errors (inter alia "delution", for dilution; "pyrophorous" for pyrophoric, etc.), grammatical errors, and worse: an unforgivable symbol error where the Greek letter ν ("nu") and the symbol for velocity (v) are used *interchangeably as frequency and velocity* (on p 57 "their velocity ν..."; on p 61 "with frequency ν and wave vector..."; on p 65 "...where $E = m\nu^2/2$.")! Errors of various types (including pentavalent carbon, missing bonds, etc.) were found on 31 pages. The editing can be summarized with one word−*schlampig*. All foreign quotations are translated in the book, except an intriguing one ("nicht sein kann, was nicht sein darf", which roughly translated is "what is not allowed, cannot be"?).

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JA955310+

Advances in Enzymology and Related Areas of Molecular Biology. Edited by Alton Meister (Cornell University Medical College). Wiley: New York. 1994. 316 pp. $119.00. ISBN 0-471-01767-1.

This volume of Advances in Enzymology continues a tradition of providing authoritative reviews on subjects that will be of interest to scientists engaged in biological chemistry generally as well as specifically to enzymologists. The increasingly multidisciplinary nature of research in enzymology is clearly reflected in the contributions to the volume. Reviews of specific enzymes, glutathione S-transferase, cholestryl ester hydrolase, and phosphoenolpyruvate carboxykinase bracket less traditional but no less interesting topics for the series on adenosine receptors, microtubules, and α-crystallin. The series has become an indispensable asset in any institution where biochemistry is either practiced or taught. For example, the current volume contains at least a dozen examples of diagrams and illustrations that can be considered for incorporation directly into the undergraduate or graduate biochemistry curriculum.

The opening chapter by Richard Armstrong on glutathione S-transferase provides an outstanding example of the application of the modern tools of molecular and structural biology to the examination of enzyme mechanism. An informative introductory section includes a useful explanation of the classification and nomenclature systems used in this field. The review provides a synopsis of mechanistically relevant insights gained from a comparison of the solutions of the three-dimensional structures for three of the isoenzymes. Correlations are

made with observations on chimeric enzymes and with the results of site-directed mutagenesis experiments to provide a reasonable mechanistic hypothesis. The title for David Hjjar's chapter, Regulation of Cholestryl Ester Hydrolases, is a bit misleading. There is an extensive description of the factors that have been found to influence catalysis including the results of experiments on the physical state of the substrate. This clearly illustrates the unique challenges of conducting enzymology in two phases. The final section provides an overview of the cellular regulation of the enzyme by eicosanoids.

Timothy Palmer and Gary Stiles present a review of the field of research on adenosine receptors. For the uninitiated in adenosine receptor pharmacology, a definition of the agonist/antagonist abbreviations would have been helpful. There is a concise synopsis of the results bearing on the current model of the structure of the receptor followed by a description of receptor function and regulation. The chapter reads as much like a research proposal as a review because there is a long section on future directions containing numerous stimulating ideas. Daniel Purich and James Angelastro contribute a beautifully written chapter on microtubule assembly and turnover. The various models that have been proposed to account for microtubule assembly are presented and discussed. There is an explanation for the paradox of microtubule assembly and disassembly based on tubulin GTP binding and hydrolysis at the boundary where polymerization takes place. Sections relating the results of *in vitro* experiments to the cellular process draw attention to the relevance of the discoveries at the molecular level to the current understanding of biological function.

The concluding chapters present two examples of the regulation of gene expression in two quite different systems: α-crystallins and phosphoenolpyruvate carboxykinase. Christina Sax and Joram Piatigorsky provide a review of research on the α-crystallins. Introductory sections describe the distribution of these proteins beyond the lens, their expression in numerous diseases, and their relationship both structurally and functionally to the small heat shock proteins. There follows a detailed analysis of the multiple regulatory elements in control of gene expression for this family of proteins. To their credit, the authors present an unbiased view of unresolved issues. The α-crystallins afford a fairly comprehensive picture of genetic regulation because experiments running the gamut from footprinting to transgenic mice have been carried out. The volume concludes with a chapter by Richard Hanson and Yashomati Patel on phosphoenolpyruvate carboxykinase. There is an excellent historical review of research integrating a huge body of information on this pivotal enzyme for the reader. By linking the subjects of species and tissue distribution with dietary and hormonal regulation, the review provides a model for studying the consequence of a basic metabolic process as it relates to issues of health and disease. An account of research results on the regulation of genetic expression for the cytosolic phosphoenolpyruvate carboxykinase then follows, culminating in a testable hypothesis that accounts for a large number of related observations.

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JA945111A

Theoretical and Computational Approaches to Interfacial Phenomena. Edited by Harrell Lee Sellers (South Dakota State University) and Joseph Thomas Golab (Amoco Research Center). Plenum: New York and London. 1994. x + 246 pp. $85.00. ISBN 0-306-44899-8.

Adsorption at solid surfaces is key to most problems in heterogeneous catalysis, electrochemistry, and adhesion. The choice of materials to optimize the adsorptive properties for specific applications has been severely hindered by the inability to make quantitative predictions of the energetics and structures of adsorbed layers. Recent advances in the computing power coupled with improved analysis techniques now permit descriptions of extended surfaces that can be utilized in predictive fashion. The monograph edited by Sellers and Golab presents some recent developments in computation methods to described adsorption.

The monograph is a set of manuscripts that describe different aspects of adsorption including electronic structure calculations to determine energetics of adsorption and reaction energetics of small molecules, molecular dynamics of collections of molecules and large molecules at interfaces, and computer simulations for structural determinations of adsorbates. This book is principally a collection of thematic journal articles as opposed to a monograph; it represents state-of-the-art modeling efforts that were presented at a conference at the end of 1993. Unfortunately there is no introductory material to introduce the topics addressed in the various articles and how these articles fit into the broader context of computational chemistry.

Reaction dynamics on metal surfaces are presented in several different contexts. A simple empirical bond-order-conservation model was shown to give good quantitative estimates for diffusion and reaction in a variety of systems where limited data are available (H. Sellers). More detailed quantum mechanical descriptions of hydrogen diffusion on metallic surfaces was examined within the context of transition state theory, where it was found that quantum tunneling effects needed to be accounted for (S. E. Wonchoba, W.-P. Hu, and D. G. Truhlar). Density functional methods were applied to metal−metal and metal−ligand bonds, which could then be extended to described adsorption on an extended metal surface (D. R. Salahub et al.). Application of density functional methods to describe the adsorption properties of boron-substituted zeolites were also presented (M. S. Stave and J. B. Nicholas). Two articles presented molecular dynamics simulations to look at ion adsorption and charge transport at an aqueous electrolyte−metal electrode interface (M. R. Philpott and J. N. Glosli, and M. L. Berkowitz and L. Perera). These simulations included the alignment of the polar water molecules and the structure of the underlying metal electrode and have demonstrated that ion approach to the electrode is closer than previously thought. Diffusion and adsorption configurations of alkane-type molecules on metal surfaces was also modeled using molecular dynamics as a model for polymer adsorption (M. Silverberg).

The second major theme covered was to describe the details of ordering in adsorbed layers. A starting point was the simulation of solvation by supercritical solvents (G. S. Anderson, K. M. Hegvik, and M. R. Hoffmann). Simulations were able to demonstrate several different structural phase domains in self-assembled monolayer films on gold substrates (J. Hautman and M. L. Klein). These types of simulations were extended to suggest how wetting of surfaces is affected by self-assembled monolayers (D. J. Olbris and Y. Shnidman). The need for detailed structure−function interactions to describe complex systems such as blood coagulation was reviewed (M. N. Liebman). Mathematical models of reaction−diffusion models were also presented to describe the propagation of neural signals along nerve axions (M. R. Hoffmann and S. P. Müller).

The articles in this book are all well written, but they are all written like journal articles, without much background introduction. The articles are useful to researchers interested in a specific topic for the article in question. However, there is no particular benefit to have this particular collection of articles in one place. This could just as well have been an issue of the *Journal of Physical Chemistry*.

Jay Benziger, *Princeton University*

JA955248G

The Neem Tree: Source of Unique Natural Products for Integrated Pest Management, Medicinal, Industrial, & Other Purposes. Edited by Heinrich Schmutterer (Giessen U., FGR). VCH: New York. 1995. xxi + 680 pp. $125.00. ISBN 3-527-30054-6.

The neem tree has been known in India and neighboring countries for more than 2000 years. It has been the subject of three international conferences, in 1980 and 1983 in Germany and in 1986 in Kenya, and of a world congress in 1993 in India. Schmutterer is uniquely suited to edit this authoritative treatise as he has devoted his professional life to the study of neem and its products and to the encouragement of others to do the same. The book is comprised of eight chapters contributed by 47 authors from 12 countries. Most authors are from Germany (16), India (8), or the U.S. (8). Due to the frequent confusion of *Azadirachta indica*, common name neem, with the similar *Melia azedarach* L., common name chinaberry, publications more than 40 years old are unreliable and are not considered in this book. The most recent references are from 1994, with many from the period of 1990−1993. I did not find references from 1995.

The book is divided into eight chapters with numerous contributors to each chapter. The highly organized outline style is somewhat distracting; up to six numbers are used as headings. For example, 4.2.1.1.5.4 is a heading for a one sentence entry! The editor has done a masterful job of organizing the various contributions into a unified

whole. Overlap among contributions is minimal. Many contributions include very useful brief summaries. I found few errors: the citation for Bhargava *et al*., 1985, is not in the reference list on page 492; on page 489 alone is spelled olone; and in Table 6.5−3 there is a heading error. Overall, the text is remarkably error free.

Chapter 1 titled The Tree and Its Characteristics is a discussion of the taxonomy, characteristics, distribution, pests, and propagation and growth of the neem tree. It is accompanied by an excellent set of 12 plates, mostly photos by H. Schmutterer, which appear in the center of the text. Chapter 2, Biologically Active Ingredients, discusses the biologically active compounds found in neem and gives the structure of each and the likely biosynthetic relationships. This chapter will be of greatest interest to natural products chemists. Chapter 3, Effects on Viruses and Organisms, gives a systematic listing of viruses and organisms influenced by neem plant parts, products, and extracts. This chapter makes up the majority of the book, 273 pages of the 666 pages of text. Included is a very useful 21-page table which lists 413 species/subspecies of insect pests susceptible to neem products. Chapter 4, Neem Products for Pest Management, Practical Results of Neem Application Against Arthropod Pests, and Probability of Development of Resistance, reports on the past use of neem products for insect control in root and tuber crops, fruit tree pests, and stored agricultural products, as well as evaluates neem-based formulations. Most products have been introduced and developed in India, and a three-page table lists neem products currently being examined for pest management in India. The toxicity of neem products is discussed in Chapter 5. Chapter 6 discusses Various Uses of Neem Products, including uses in traditional and modern medicine, particularly as population control agents, uses in agriculture as nitrification inhibitors and manure, uses as animal feeds, and uses in soap making. The vast majority of the neem products discussed are used in India. Chapter 7 contains information rarely included in scientific treatises: Economic, Socioeconomic and Policy Considerations, and Neem in Sociocultural Life in South Asia. In Table 7.1−2 an estimation of production cost of soap from neem included the incredible estimate of 40 person days of labor @ $1.50 per day. The numbers come from a 1992 reference. This chapter will have only limited international use. Chapter 8 provides very useful discussion of other Meliaceous plants possessing bioactive ingredients.

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JA9553112

Chemical Nomenclatures and the Computer. By D. J. Polton (University of Hull, U.K.). John Wiley & Sons Inc.: New York, Chichester, Toronto, Brisbane, and Singapore. 1993. xii + 264 pp. $74.95. ISBN 0-471-94239-1.

The book of D. J. Polton on *Chemical Nomenclatures and the Computer* I found to be both interesting and very informative. At first, however, it was a difficult book to sit down and begin reading. This was due primarily to the subject material. But once I got past about the first chapter, I found myself drawn more and more into the subject matter, much like one would get drawn into solving a puzzle. A large part of this book concerns the interconversion of chemical structures into one of four types of nomenclature and/or notation; IUPAC into Dyson nomenclature, into Lozac'h nodal nomenclature, into the HIRN system of nomenclature, and into the path connectivity matrix (PCM).

Chapter 1 is devoted primarily to a review of current nomenclatures and a brief description and summary of some of the many nomenclatures and notational systems which have been proposed and developed over the past 50 or so years. Some of the more noteworthy systems briefly mentioned are, of course, the IUPAC nomenclature as well as the IUPAC notation, the Wiswesser line notation (WLN), the Dyson nomenclature/notation, Nodal nomenclature, the HIRN system, the Concise Connection Table (CCT), Structural fragments codes, the Line formulae notation, and the DARC system.

Chapters 2−7 deal primarily with applications of the various types of nomenclatures and notations. A large percentage of the book is devoted to converting chemical structures and/or IUPAC nomenclature into the Lozac'h nodal nomenclature, HIRN nomenclature, Dyson nomenclature, and the path connectivity matrix (PCM). This part of the book actually became entertaining in that it was a challenge to see if I could correctly make the various conversions. In many ways, it was like solving a crossword puzzle.

As we discover more and more molecules and are able to determine their structures, it will become increasingly important that we use systems of nomenclature that are compatible with computer storage. Three-dimensional representation of structures will also become essential. As Dr. Polton states, "it will be advantageous to have, at some time, a way of naming compounds which does not need a reference book of more than 500 pages". He also predicts that "Programs will become of minimum complexity and new systems, of nomenclature or what-else, will be of an easy construction as possible". This book, I believe, will help speed along this construction process.

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JA934828F

Combustion Efficiency and Air Quality. Edited by Istvan Hargittai (Budapest Technical University, Hungary) and Tamas Vidoczy (Hungarian Academy of Science, Hungary). Plenum Press: New York. 1995. xiii + 289 pp. $85.00. ISBN 0-306-44848-3.

This volume is a strange mix, assembled under the title above. The book is based on a workshop held in 1993 at the Institute of General and Analytical Chemistry of the Budapest Technical University. Topics discussed during the workshop ranged from molecular structure and energetics, elementary reactions, kinetic modeling, combustion theory, and combustion in practical systems to emission analysis and control, atmospheric chemistry, and waste incineration.

Most of these topics are discussed in this monograph, though it would be difficult to see why several should be under this title. In addition, there is a great diversity in quality and depth between the different chapters. Topics in the different chapters include subjects such as the Club of Rome and the development of the flame ionization detector (Chapter 1); detailed analysis of nitrogen oxides and nitro compounds bond angles (Chapter 2); preparation, structure and bonding, energetics, and detonation characteristics of covalent inorganic non-metal azides (Chapter 3); as well as fluidized bed combustion (Chapter 7); studies of fly ash particles (Chapter 11); and damage assessment (Chapter 14).

Chapter 7 (on clean combustion utilizing fluidized-bed boilers) is entirely qualitative, touching on numerous topics in 13 pages and citing only three references, none of them readily available. Any reader desiring to learn the state-of-the-art on this topic from a fundamental perspective would be better off to peruse recent volumes of the International Combustion Symposia. The short Chapter 9 on incineration on waste solvents contains some useful information as well as critical observations. It would have been profitable if the authors had elaborated on some points, such as the kinetic compensation effect. Measurements of PCDD/F in incinerators have improved considerably since the 1987 reference cited. By comparison Chapter 10—dealing with combustion in particles in outdoor and indoor environments—seems far too long. And there is yet another chapter on indoor air quality (Chapter 13). Chapter 6 gives a theoretical quantum-mechanical study of soot formation, i.e., ab initio calculations are emphasized. Chapter 11 is a comprehensive compilation of instrumental methods that have been brought to bear on the bulk and surface analysis of fly ash particles. This chapter could have been made more valuable by a critical analysis comparing the pro's and con's of each technique. It is also surprising that there was no reference to the work of T. Eighmy. Chapter 5 discusses the partial oxidation of methane, but chiefly from a C_2-synthesis point-of-view.

It is unlikely that this book will be considered a primary or introductory reference to any of the topics covered. The theoretical chemist, the combustion engineer, the specialist interested in ambient air sampling, and the policy maker would each find perhaps two to three chapters of interest. The purchase price of $85.00 further would discourage acquisition for the personal library.

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