

Additions and Corrections

Theoretical Studies of *o*-, *m*-, and *p*-Benzyne Negative Ions [*J. Am. Chem. Soc.* **1996**, *118*, 11872–11883]. JOHN J. NASH AND ROBERT R. SQUIRES*

An error in one of the exponents of the basis set used for the B3LYP/cc-pVTZ calculations led to incorrect total energies for the benzyne anions, benzene, phenyl radical, and phenyl anion. The correct B3LYP/cc-pVTZ total energies are given below, along with amended values of the thermochemical data that were

derived from these energies. Because the basis set error was the same in the calculations for all six molecules, the derived thermodynamic quantities are essentially the same as those listed in the paper, and all the qualitative conclusions are unchanged. The explanation given on page 11881 for the lower B3LYP/cc-pVTZ energies relative to the B3LYP/cc-pVDZ energies as a result of the non-variational nature of the B3LYP method, while possible in principle, is incorrect in the present case.

Table 1. Corrections for Tables 3, 4, and 7: B3LYP/cc-pVTZ Energies for *o*-, *m*-, and *p*-Benzyne Anions, Benzene, Phenyl Radical, and Phenyl Anion (au); Calculated Relative and Absolute Proton and Hydrogen Atom Affinities of Benzyne Anions (kcal/mol)

	² B ₂ <i>o</i> -benzyne anion	² B ₂ <i>m</i> -benzyne anion	² A _g <i>p</i> -benzyne anion	benzene	phenyl radical	phenyl anion
E_{TOT} B3LYP/cc-pVTZ ^a (6d, 10f)	-231.02027	-231.01085	-231.00224	-232.33694	-231.64763	-231.67711
H_{rel} (298 K)	0.0	6.3	11.5			
$\Delta H(\text{eq } 3)^b$	19.6	14.0	9.1			
$\Delta H_{\text{acid}}(\text{C}_6\text{H}_5)^c$	382.1	387.7	392.6			
$DH_{298}[\text{C}_6\text{H}_4^- - \text{H}]^d$	93.9	99.5	104.4			

^a Total energies computed for B3LYP/cc-pVDZ geometries; cc-pVTZ basis set includes six d-functions and ten f-functions for carbon. ^b Enthalpy change at 298 K for proton transfer from benzene to benzyne anion. ^c Gas-phase acidity of phenyl radical at the *ortho*, *meta*, and *para* positions, respectively. ^d CH bond enthalpy of the phenyl anion at the *ortho*, *meta*, and *para* positions, respectively.

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Book Reviews *

Biomarkers in Food Chemical Risk Assessment. Edited by Helen M. Crews and A. Bryan Hanley (CSL Food Science Laboratory, Norwich, U.K.). The Royal Society of Chemistry: Cambridge, 1995. £45.00. x + 138 pp. ISBN 0-85404-790-5.

This book comprises a collection of thirteen papers presented at the Biomarkers in Food Chemical Risk Assessment Symposium, held on March 1–3, 1995, at CSL Food Science Laboratory, Norwich Research Park, U.K. The objective of the symposium was to recognize the need for and begin the development of a multidisciplinary understanding of food chemical risk assessment. It is generally recognized that diet contributes significantly to human diseases, but the understanding of the specific roles of dietary factors and pathways to their effect(s) is murky at best.

This book makes no pretense of absolutely clearing the murkiness, but maps a clear strategy for the multidisciplinary approach that the preface to the book calls for. Contributing disciplines include food science (the preponderance of contributions), toxicology, biochemistry, clinical sciences, and oncology. The papers range from general overviews to specific case studies. The collection is “book-ended” by general summaries and proposals for study in the biomarkers field, while the remainder of papers are more specific (case studies and the like). Exposure biomarkers, effect (response) biomarkers, and susceptibility biomarkers are discussed in the proceedings. The authors deal not only with difficulties in the scientific methods, but also emphasize the difficulties in interpretation, extrapolation, and application of data. The approach to methodology is strong.

Specific topics covered in the text include food chemicals and contaminants, artificial sweeteners, dietary minerals, toxic chemical exposure, antioxidant effects, genotoxic agents, DNA adduct analysis, and heterocyclic aromatic amines. Most of these topics are covered by scientifically sound presentations. The references date mainly from the 1980s and the early 1990s, which is viewed as appropriate for the publication date of these proceedings.

The editing of the collection is well-done. The stylistic presentation of the papers and their progression provide pleasant, informative study.

*Unsigned book reviews are by the Book Review Editor.

As a reviewer whose main research is somewhat outside this field, I found the book to be interesting, highly informative, and an excellent resource for someone interested in beginning investigations in this field.

Daina Briedis, Michigan State University

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Polymer Syntheses, Volume III, Second Edition. By Stanley R. Sandler (ELF ATOCHEM North America, Inc.) and Wolf Karo. Academic Press: San Diego. 1996. xiii + 424 pp. ISBN 0-12-618513-1.

This book is the welcome complement to the second editions of Volumes I and II (1992 and 1994, respectively). The text is much the same as that of the first edition, but it has been updated with significant new references and an expanded final chapter on miscellaneous methods. Fully one-fourth of the end-of-chapter citations date since the publication of the first edition, most of these just since 1990.

The text appears to have been edited somewhat casually. There are inconsistencies in verb tense in a number of the procedures (*e.g.*, pp 316, 320, 339, and 378), and subject/verb number agreement is not always maintained (pp 323, 344, 409, and 410). “Ideal” is used in place of “idea” (p 382), and two different spellings of “liter” are used in the same sentence on p 404. Typographical errors in chemical terms such as “acetaone”, “tiallyl citrate”, “tetraabutylamonmonium bromide”, and “eluding solvents” (pp 317, 322, 377, and 409) will likely cause little confusion to knowledgeable chemists, as will “hypochloride” for the Hofmann rearrangement (p 399) or the formula $\text{RhC}_{13}\cdot 3\text{H}_2\text{O}$, which is intended to represent the rhodium(III) chloride salt (p 391).

The functional value of this work is little diminished by such solecisms and misspellings. The authors have provided a valuable summary of a wide range of synthetic methods. Typical procedures for the syntheses of olefin–sulfur dioxide copolymers, polythioethers, sulfide polymers, polyisocyanates, poly(oxyalkylhydroxy) compounds,

polyvinylcarbazole, poly(vinyl acetate), poly(allyl esters), and poly(vinyl fluoride) have all been updated in this second edition with current references to the journal and patent literature, and additional emphasis has been placed on their associated hazards. Notable additions to the final chapter on miscellaneous polymer preparations include brief descriptions of polymers from propargyl-terminated monomers, polycyanurates, starburst dendrimers, metal-containing polymers for catalysis, monodisperse latices, optically active polymers, and techniques of polymerization in supercritical fluids, and even a very short section on polymers based on fullerenes. There are, however, no descriptions of syntheses of polythiophenes, polypyrroles, polyanilines, or other such materials that are noted for their high electrical conductivities.

This book is a valuable reference work for specialists and nonspecialists alike. It is an excellent place to begin a search for a reliable synthetic method.

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JA965796+

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DNA Sequencing Strategies: Automated and Advanced Approaches. Edited by Wilhelm Ansorge, Hartmut Voss, and Jürgen Zimmermann (EMBL, Heidelberg). Wiley: New York. 1996. xiv + 202 pp. \$39.95. ISBN 0-471-13683-2.

This book is the first in a series of practical books designed by EMBO, the European Molecular Biology Organization. Each year, EMBO supports approximately 20 practical courses in all parts of Europe, with the goal of facilitating access of European researchers to recent scientific developments. Since only 20 participants are selected for each course, EMBO has decided to publish the material covered in the courses as practical manuals in order to reach a wider cross-section of the scientific community. The first book in this series deals with strategies for large-scale DNA sequencing.

The book is essentially a laboratory manual consisting of five chapters. Chapter 1 provides protocols for cloning DNA. The topics include construction of shotgun libraries of randomly sheared DNA, methods for shotgun cloning of fragments derived from partial cleavage of DNA with restriction enzymes, production of nested deletions, methods for introducing DNA in bacteria for amplification, and an overview of selected cloning vectors and *E. coli* strains used as hosts in cloning experiments. Chapter 2 covers selected procedures for preparing plasmid DNA and for isolating human genomic DNA for amplification by PCR. This chapter also includes strategies for processing the PCR products to prepare templates suitable for DNA sequencing. Chapter 3 goes over various strategies used for sequencing DNA. They include sequencing double- and single-stranded DNA, utilization of fluorescence dyes, cycle sequencing protocols, and automated DNA sequencing. Chapter 4 gives an in-depth coverage of methods for preparing primers for sequencing reactions, strategies for primer selection, and the chemistry underlying the automated machines for DNA synthesis. Chapter 5 outlines the steps in preparing gels and electrophoretic analysis of DNA for sequence determination. Chapter 6 glides rapidly over computational methods for data interpretation including fragment assembly and DNA sequence analysis.

Overall, the book provides a reasonable cross-section of up-to-date strategies for sequencing DNA. The book is concise and yet relatively easy to follow. It could be a valuable asset to graduate students interested in learning about DNA sequencing and a valuable resource for individuals interested in including, in instructional courses, representative examples of methods for DNA sequence determination and analysis.

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Photothermal Spectroscopy Methods for Chemical Analysis. Chemical Analysis Series, Volume 134. By Stephen E. Bialkowski (Utah State University). Wiley: New York. 1996. xxix + 584 pp. \$89.95. ISBN 0-471-57467-8.

This volume in the Chemical Analysis Series provides an authoritative and complete overview of photothermal spectroscopic methods, and their application to detection and analysis. Photothermal spectroscopy concerns the measurement of heat deposited in a sample by absorption of light, providing a high-sensitivity, indirect measurement of weak optical absorption useful in trace-level spectroscopic detection.

The book begins with a clear physical description of photothermal phenomena and brief history of early applications to spectroscopy and analysis. Having motivated the reader with a basic understanding of the measurement, Bialkowski next presents a thorough and well-organized coverage of the physical processes that govern photothermal measurement: these include photoexcitation (including both linear and nonlinear absorption), excited-state relaxation kinetics that govern the yield and rate of heat generation, hydrodynamic relaxation of the sample (heat-transfer and acoustics) in response to transient heating, and finally the principles of optics needed to understand optical probing of thermally-induced refractive index gradients in the sample. In subsequent chapters, Bialkowski combines these physical processes to describe heat-induced optical elements produced in a sample, and the design and response of photothermal spectroscopies, particularly beam-deflection and thermal-lens measurements. Analytical applications of photothermal spectroscopy for detecting weak optical absorption in both gas and liquid phases and in heterogeneous samples are surveyed, along with a short summary of measurements of excitation and decay kinetics and quantum yields.

The major contribution of this book is in providing a complete theoretical description of the physics underlying photothermal measurements. The subject is diverse, requiring background in many fields including photophysics, heat transport, optics, and signal processing. This book presents a complete and well-organized coverage of these areas so that the principles and practice of photothermal spectroscopy methods can be readily understood.

Joel M. Harris, *University of Utah*

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The Chemistry of the Atmosphere – Oxidants and Oxidation in the Earth's Atmosphere, 7th BOC Priestley Conference. Edited by A. R. Bandy (Drexel University). The Royal Society of Chemistry: Cambridge. 1995. viii + 228 pp. £55.00. ISBN 0-85404-765-4.

This book provides a general and revealing overview of recent research in atmospheric chemistry. A panel of world experts, including 1995 Nobel Laureates Paul Crutzen and Mario Molina, characterize four major areas of concern: the oxidative fate of atmospheric pollutants; urban and regional photochemical pollution; trends in global tropospheric ozone levels; and stratospheric ozone depletion mechanisms. This book also contains a section entitled *The Early History of Ozone*. It includes discussions involving Schönbein, Faraday, Berzelius, and Liebig and provides insight into historic scientific thought on a molecule which is much in the news today.

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