Additions and Corrections

Molecular Charge Distribution, Core-Ionization Energies, and the Point-Charge Approximation [*J. Am. Chem. Soc.* **1991**, *113*, 5224]. LEIF J. SAETHRE,* MICHELE R. F. SIGGEL,* and T. DARRAH THOMAS*

Professor Bader has pointed out to us that some of the results presented in this paper do not represent predictions of the atoms-in-molecules model. The wave functions we have used produce a maximum in the electron density (pseudoatom) between the two carbons in ethene and the halogenated ethenes. The division of the molecules into basins has involved boundaries drawn from this maximum rather than from a saddle point (as required by the atoms-in-molecules approach). We have repeated our calculations for ethene and fluoroethene with the 6-31G** basis set, which produces only a saddle point between the carbons. From these calculations, we find that our conclusions about the lack of validity of the point-charge model are unchanged. A summary of these additional calculations is in press: Saethre, L. J.; Siggel, M. R. F.; Thomas, T. D. *J. Electron Spectrosc.*, in press.

Homolytic Bond (H–A) Dissociation Free Energies in Solution. Applications of the Standard Potential of the $(H^+/H^\bullet)$ Couple [*J. Am. Chem. Soc.* **1992**, *114*, 7458–7462]. VERNON D. PARKER

The standard state for the thermodynamic data in Table I is pure gas (unit mole fraction). The data should have been converted to unit activity standard state for use in Table II. Also, recent experimental data (Roduner, E.; Bartels, D. M. *Ber. Bunsenges. Phys. Chem.* **1992**, *96*, 1037–1042) suggest that H_2 is a better model for the hydrogen atom than He for the estimation of the free energy of solvation.

Page 7460, Table II: column 2, −0.87, −0.17; column 3, −2.29, −1.77, −2.48; column 4, −2.29, −2.24, −2.28.

Page 7461, Tables III and IV: ΔG_{hom} in H_2O should be decreased by 3.00 kcal/mol.

Page 7461, Table V: ΔG_{hom} in DMSO should be decreased by 2.30 kcal/mol.

Page 7461, Table VI: ΔG_{hom} in acetonitrile should be decreased by 2.54 kcal/mol.

I am grateful to Drs. David M. Bartels and Emil Roduner for calling these errors to my attention.

Computer Software Reviews

JMPIN. Version 1.0.6. SAS Institute Inc.: SAS Campus Drive, Cary, NC 27513. 1992. List price $39.95.

JMPIN is an introductory version of JMP 2.0 (see previous review) that is intended for students and demonstration use only. Included in the software package is the application (600K), help files (340K), and a Sample Data folder (171K). The operations in JMPIN are analogous to those found in JMP 2.0 with a few exceptions. Most of the differences are quite minor with the exception that saving, importing/exporting, and cutting/pasting files are limited to 500 data cells. JMPIN allows the user to analyze larger data tables, but once more data cells are created or entered they cannot be saved directly. Obviously this restriction intentionally impairs full operation of the program with large data sets and should be taken into consideration by potential users. Even with these restrictions, JMPIN is well suited to handle most of a student's statistical problems at a very reasonable price.

Kraig A. Wheeler, *The University of Texas at Austin*

JMP. Version 2.0.4. SAS Institute Inc.: SAS Campus Drive, Cary, NC 27512. 1992. List price $695.00 ($347.50 Academic).

JMP is a statistical graphics package for Apple Macintosh computers. In brief, the program allows for editing, transforming, and viewing along with statistical analysis of numerical and character data. The most notable feature of the program is its ability to analyze data statistically. In addition to the software, the package comes with a detailed user's guide which provides the needed support to the different JMP options.

The program is shipped on two 3.5 in. double-sided double-density disks that are not copy protected to allow for personal backup copies. The uncompressed application (1175K) and help files (616K) are retrieved from a Stuffit Archive format with the appropriate application supplied with the software. Also included in the software package is a Sample Data folder (469K) used as a teaching tool for the various graphics features and statistical platforms. One megabyte of memory is required to run the program; however, two megabytes are recommended. JMP Version 2.0 is compatible with any Apple Macintosh computer and System Software Version 6.0 or later; this is a drastic improvement from Version 1.0.

The documentation for JMP (722 pages) is an invaluable tool when one is first becoming familiar with the program. The program does allow for the new user to proceed without review of the user guide which is recommended anyway due to the extensive features and abilities of JMP. A thorough understanding of the documentation is necessary before full application of the program can be realized. The documentation is divided into two sections. The first section (introductory guide) is a collection of tutorials designed to help the user learn JMP strategies. Each tutorial uses a file from the Sample Data folder. By following through these step-by-step processes, the user can quickly become familiar with the JMP menus, options, and report windows. The tutorials range from single step procedures to complex analyses. The second section (user's guide) contains complete documentation of all JMP menus and an explanation of data table manipulations. These chapters describe how common tasks such as manipulating files, selecting subsets, transforming data table columns, and cutting and pasting JMP data and analyses can be achieved. Additionally, this section describes each of the statistical platforms, report windows, and options in detail. References and brief discussions are also available for each computational method to help the user understand how statistical results are obtained and interpreted.

Importing data is accomplished by reading data from a JMP export file, SAS transport file, or standard text file. The format of the incoming file can be accommodated by specifying the approprite end-of-field and end-of-line delimiters. Once the data have been imported into JMP's spread sheet, data columns and rows can be altered or created. Standard file operations are available as well as several other options (i.e., calculator, subset, sort, join, concatenate, stack, and transpose).

Even though JMP is not primarily a graphics program, the software package provides many plotting features. The more notable of these features are color plots, overlay plots, confidence curves, and pareto charts. JMP has commands that represent eight statistical platforms: distribution of Y's, fit Y by X, fit Y by X's, specify model, nonlinear fit, spin, Y's, by Y's, and special graphs. The various statistical parameters associated with these platforms are too numerous to list here, but include multiple regressions, nonparametric tests, factor analyses, and distributions. Each of the statistical methodologies ranges from simple to complex and has a wide variety of applications. The statistical approach of each platform is well documented and referenced, presented in the user guide and through the help menus. Because interpretation of the results is necessary, it is recommended that the user have a minimal background in statistics in order to get full use of the programs statistical package.

JMP provides a powerful statistical tool with capabilities that typically exceed what the average scientist or student would need. The program is versatile and user friendly, allowing both the trained professional and the novice to design specific statistical analyses. JMP is a solid program and worthy of consideration by the scientific community.

Kraig A. Wheeler, *The University of Texas at Austin*

*Book Reviews**

Chemical Industries Series. Volume 47. Catalysis of Organic Reactions. Edited by William E. Pascoe (Eastman Kodak Company). Marcel Dekker: New York. 1992. xvi + 386 pp. $150.00. ISBN 0-8247-8573-8.

This volume is a collection of the papers and posters presented at the Thirteenth Conference on Catalysis of Organic Reactions in Boca Raton, Florida, in May 1990. The book is in two sections "Reactions with Hydrogen" and "Other Catalytic Reactions in Organic Synthesis", which contains subsections on "Acid-Catalysis", "Dehydrogenations", "Oxidations", and "Special Topics in Catalysis".

The subject matter in this book covers a broad range of research that is of interest to the chemical community. The sizable contribution from academia (approximately 40%) to this book demonstrates this overlap in research interests. However, there is a large imbalance in the coverage given each subject. The area of research with by far the largest influence in this book is the use of supported metal catalysts for heterogeneous hydrogenation and dehydrogenation reactions (15 chapters out of 33). Throughout the book many examples illustrate the variety of the research industrial chemists perform on all aspects of heterogeneous catalysis, such as catalyst structure, selectivity, by-product formation, reaction modeling, reaction vessel design, catalyst poisoning, and reactivation. Several important areas of industrial research only receive scant attention in this book, including such topics as enzymes in industrial processes (1 chapter), zeolites (2 chapters), phase transfer catalysis (1 chapter), and chiral synthesis (1 chapter); this imbalance in subject material is the major failing of this current publication.

This volume contains over 500 references, with a sizable number of recent citations. However, over half of the citations appear in only six chapters, and there are no fewer than sixteen chapters that contain ten or fewer references (three of the chapters contain no citations at all). No doubt, this is partially due to the inclusion of chapters based on the poster sessions from the conference.

In summary, this book provides an insight into industrial research problems, although the price and variety of subject material mean that purchasing of this volume will only be of interest to libraries and specialists in the field.

Andrew Bennet, *Simon Fraser University*

The Total Synthesis of Natural Products. Volume 9. The Synthesis of Insect Pheromones, 1979–1989. By Kenji Mori. Edited by John ApSimon. John Wiley & Sons: New York. 1992. ix + 533 pp. $125.00. ISBN 0-471-55189-9.

John ApSimon has been the editor of this most valuable series of compilations of organic syntheses since its inception in 1973. After 18 years of exceptional service to the organic community, he has now decided to pass the responsibility to another editor. Volume 9 of this series maintains the standard which has typified successive volumes down the years and should stand as a final tribute to his endeavors. The current volume is the work of a single author, Professor Kenji Mori, and documents, in a comprehensive way, the extensive synthetic effort associated with insect pheromones through its most productive time from 1979 to 1990. The book is a tour de force from Professor Mori, but its painstaking and lucid description of the field will come as no surprise to those familiar with the dedication which the author brings to all of his projects. The syntheses of no fewer than 260 pheromones have been reviewed in the book, which contains 987 schemes and delineates 1229 references. It will surely be unnecessary to review the field again the foreseeable future.

Of the possible approaches available, the author has chosen to classify the pheromones according to structural type and enantioselective synthesis has been included in each section rather than in a separate chapter. The main body of the work is preceded by a short, but valuable, review of a number of general methods for the synthesis of pheromones. Thus the alkylation of acetylenes, Wittig reactions in a heterogeneous medium, olefin inversion, and other procedures are delineated. The treatise then deals successively with alkanes, olefins, unsaturated alcohols and acetates, conjugated dienes and enynes, trienes and tetraenes, epoxides, chiral alcohols, aldehydes, ketones, lactones, isoprenoid derivatives, oxygen heterocycles, acetals, and spiroacetals. The descriptions, whilst precise, give a wealth of information which can be readily assimilated by either the casual or more serious reader. Reagents and conditions for individual procedures are clearly listed together with yields of reactions to allow judgement to be made on the attractiveness of the approach. In enantioselective syntheses, the optical rotation of the final pheromone is included in the schemes and care has been taken to discuss information on the enantiomeric excess of the products in a critical fashion.

To those of us who took part in the development of this chemistry, the book is a timely reminder of some of the excitements of the period. Expectations that pheromones might play a major role in insect control systems have not been fulfilled, but the chemistry engendered in the period has added a significant number of processes to our synthetic libraries, many of them capable of being transferred to large scale operations. The sections on enantiomeric syntheses are also of real value and allow direct comparison to be made of alternative procedures. For example, seven asymmetric syntheses of frontalin are described, three of which employed asymmetric carbon-carbon bond forming reactions. The intricacies of enantiomeric specific syntheses of spiroacetals are also noteworthy.

The most impressive aspect of the book is the clarity in which the synthetic schemes have been described. Professor Mori has been meticulous in the detail provided, and the important aspects of the schemes are readily appreciated by the reader. It is a book that can be enjoyed by those who wish to dip quickly into the various sections or by the more serious reader to garner information for his purposes. It will rapidly attain the status of the reference text for nearly two decades of chemistry, and deservedly so. The author has, indeed, transferred his immense knowledge and expertise from the laboratory to an outstanding piece of scholarship to the benefit of all involved in the art of organic synthesis. The book can be recommended, wholeheartedly, to those who will make regular reference and also to libraries where the book will soon be regarded as the masterpiece which it is.

Raymond Baker, *Merck Sharp & Dohme Research Laboratories*

Chemical Analysis. Volume 115. Trace and Ultratrace Analysis by HPLC. By Satinder Ahuja (Ciba Geigy Corporation). Wiley-Interscience: New York. 1992. xi + 419 pp. $75.00. ISBN 0-471-51419-5.

This book on trace analysis using HPLC is the latest addition to the excellent *Chemical Analysis* series. The author indicates that his goal is to provide solutions to real problems and to open new doors to knowledge. To accomplish these goals, the book presents basic theory, discusses instrumental considerations in trace analysis, provides an overview of sample preparation and method development, and reviews many applications. The latter comprise nearly 25% of the book. The index is relatively good in directing the reader to the specifics of a method, an absolute necessity for this type of book.

The presentation of theory is accurate and understandable, but not novel. The nearly word for word repetition of the equations and discussion from pages 56–57 on page 165 leads this reviewer to conclude

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*Unsigned book reviews are by the Book Review Editor.