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.

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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.