Additions and Corrections

Solution Homolytic Bond Dissociation Energies of Organo-transition-Metal Hydrides [*J. Am. Chem. Soc.* **1989**, *111*, 6711]. MATS TILSET* and VERNON D. PARKER*

Page 6712: The constants 45.6 in eq 12 and 50.3 in eq 15 are in error by 8.0 kcal/mol and should read 53.6 (eq 12) and 58.3 (eq 15). Consequently, the M–H BDE in Table II should be 8 kcal/mol greater than indicated. The electrode potentials used in the equations are referred to the (H^+/H_2) electrode in acetonitrile. When using this potential scale no correction for the free energy of transfer of the proton from acetonitrile to water is necessary. This correction was erroneously made in eq 12 and 15. The relative values of the BDE in Table II are not affected by the correction.

^{15}N Chemical Shifts of Backbone Amides in Bovine Pancreatic Trypsin Inhibitor and Apamin [*J. Am. Chem. Soc.* **1989**, *111*, 7716–7722]. JOHN GLUSHKA, MARIA LEE, SCOTT COFFIN, and DAVID COWBURN*

Page 7719, Table III: The values were not calculated correctly for the model discussed in the text. The revised Table III is presented with the changes in columns 2, 3, 4, 5, and 6. The values for Arg, His, Lys, and Pro have been changed in column 2. In addition, the values for the *N*-acetyl amino acids in column 2 have been referenced where appropriate.

Page 7718, Table I: $\Delta\delta^{15}$N values for the following residues are corrected—G12 (–4.1), K15 (–10.5), F33 (–3.4), G36 (+2.9), R39 (–13.1), K41 (–2.9), S47 (–8.7), C55 (–6.3), G57 (–0.5). The δ^{15}N value for S47 is 108.8 ppm.

Page 7718, Table II: The $\Delta\delta^{15}$N values in column 7 should be Asn-2 (+3.7), Cys-3 (–0.6), Lys-4 (–6.2), Ala-5 (–6.3), Glu-7 (–0.3), Thr-8 (–5.0), Ala-9 (+0.3), Leu-10 (–2.5), Cys-11 (–4.0), Ala-12 (–2.7), Arg-13 (–7.2), Arg-14 (–5.9), Cys-15 (–4.4), Gln-16 (–4.8), Gln-17 (–4.7), His-18 (–4.1).

Page 7720, Table IV: Two values, for F33 and G36, taken from Table I should be changed to agree with the corrected values in Table I (F33, –4.9 → –3.4; G36, +1.9 → +2.9).

Page 7720, paragraph 6, bottom right column: The corrected values for A9 and R13 should be used in the text, and the reference to A12 deleted. The paragraph should read as follows—A similar comparison of the apamin data (pH 2.2) to random-coil chemical shift values reveals the same wide variation. For example, A9 ($\Delta\delta^{15}$N = +0.3) is downfield, which is compatible with participation in multiple hydrogen bonds.[33,53] However, R13, C11, L10, and Q16 all have similar hydrogen bond patterns and yet are all relatively upfield. R13 in particular is a donor amide and the preceding carbonyl of A12 is an acceptor, yet it is 7.2 ppm upfield of its random-coil value.

Page 7722, left column, lines 9–15 T8 should be T11 in both instances, and the value for S47 should be 8.7. Thus sentences 2 and 3 should read as follows—For example, T11 and S47 have shift differences from their random coil analogues of 14.9 ppm downfield and 8.7 ppm upfield, respectively. However, a 7-Å radius around each amide shows very similar environments in terms of distances from the nitrogens to aromatic groups, carbonyl

Table III. ^{15}N Chemical Shifts of *N*-Acetyl Amino Acids[a] and Random Coil Peptides[b]

| residue$_i$ | *N*-acetyl | neighboring residue$_{i-1}$ | | | |
		Gly,Ala	β-methylene[c]	Val	Ile
Ala	125.7[d]	124.3	126.2	127.7	128.7
Arg	126.1[e]	124.7	126.6	128.1	129.1
Asn	123.2[f]	121.8	123.7	125.2	126.2
Asp	121.6[e]	120.2	122.1	123.6	124.6
Cys	120.6[g]	119.2	121.1	122.6	123.6
Gln	123.7[f]	122.3	124.2	125.7	126.7
Glu	122.0[e]	120.6	122.5	124.0	125.0
Gly	110.7[d]	109.3	111.2	112.7	113.7
His	123.2[h]	121.8	123.7	125.2	126.2
Ile	120.6[g]	121.1	123.0	124.5	125.5
Leu	123.3[g]	121.9	123.8	125.3	126.3
Lys	125.5[h]	124.1	126.0	127.5	128.5
Met	121.6[e]	120.2	122.1	123.6	124.6
Phe	122.3[e]	120.9	122.8	124.3	125.3
Pro	132.4[g]	131.0	132.9	134.4	135.4
Ser	117.0[e]	115.6	117.5	119.0	120.0
Thr	111.9[e]	110.5	112.4	113.9	114.9
Trp	123.6[e]	122.2	124.1	125.6	126.6
Tyr	123.4[f]	122.0	123.9	125.4	126.4
Val	119.3[d]	119.8	121.7	123.2	124.2

[a] *N*-Acetyl amino acids in DMSO, ppm relative to NH_3. The values for Arg, His, Lys, and Pro have been corrected from the original table. [b] Calculated values for random coil peptides in H_2O, ppm relative to NH_3. [c] All residues containing a side chain β-methylene, i.e. Asp, Asn, Glu, Gln, Arg, Lys, Phe, Thr, Tyr, Trp, His, Leu, Ser, Pro, Met, Cys. [d] Values from ref 1. [e] Measured in DMSO. [f] Values from ref 4. [g] Values from: Hawkes, G. E.; Randall, E. W.; Bradley, C. H. *Nature* **1975**, *257*, 767–772. [h] Measured in H_2O; DMSO value calculated with –5.7 ppm correction based on measured differences for NAcAla and NAcArg in DMSO and H_2O.

groups, and other amides, although the S47 amide is in a more hydrophobic environment with less accessible surface area than the T11 amide.

σ-Bond Metathesis Reactions of Si–H and M–Si Bonds. New Routes to d^0 Metal Silyl Complexes [*J. Am. Chem. Soc.* **1989**, *111*, 3757]. HEE-GWEON WOO and T. DON TILLEY*

The compounds CpCp*ZrHCl and CpCp*HfHCl are incorrectly reported to be dimeric. Solution molecular weight measurements (in benzene) are actually more consistent with monomeric structures.

Dehydrogenative Polymerization of Silanes to Polysilanes by Zirconocene and Hafnocene Catalysts. A New Polymerization Mechanism [*J. Am. Chem. Soc.* **1989**, *111*, 8043]. HEE-GWEON WOO and T. DON TILLEY*

The compounds CpCp*ZrHCl and CpCp*HfHCl are incorrectly reported to be dimeric. Solution molecular weight measurements (in benzene) are actually more consistent with monomeric structures.

Computer Software Reviews

LabSolutions. The Center for Science Support, Inc.: 54 Brattle Street, Arlington, MA 02174. List Price $90.00.

LabSolutions is a collection of five programs that could be very useful to the student but is especially useful to chemists that are continually preparing various types of solutions. The programs include the following: The Solution Formulator, The pK Adjuster, The Serial Diluter, The Mixer and Diluter, and The Molecular Weight Calculator. The software also includes the following data tables: The Elements, The Chemical Tables, The Buffers, and The Strong Acids and Bases. The user can add, edit, or delete data in the chemical and buffer tables.

LabSolutions is copyrighted and supplied on registered disks. The Center for Science Support, Inc. does authorize the user to make archival copies for backup. The software can be used on IBM PC/XT/AT, PS/2 or compatible Computers (DOS 2.1 or higher) with a single floppy or hard disk, 256 K RAM, and with monochrome or color monitors.

The software is extremely user friendly. The novice can quickly master this software with the use of the manual and the prompts. In the event of a problem, the publishers are very courteous and helpful in answering questions. The software allows laboratory personnel to organize their customized files into separate subdirectories for direct retrieval.

LabSolutions comes with an excellent User's Manual. First of all, it contains easy step-by-step instructions for each of the five programs with examples. It also contains an explanation of each of the pop-up data tables stating how the table was prepared, how it is to be used, and how to add, delete, or edit information in the table. In the appendix, there is a section that explains the equations and the calculations used for the acid, base, and buffer formulations. As an additional reference for the chemist, the manual gives suggestions on the proper procedures to follow during solution preparation, including safety hints. There are also recipes for standard buffers showing the amounts of the acid/base forms to be added to obtain a given pH value.

The Solution Formulator program is limited in scope in acid–base calculations when compared to The Acid–Base Program For Chemistry (by R. W. Ramette, Carleton College, available from Flexible Software, Northfield, MN). In The Solution Formulator program, the chemist has to pick the acid–base or buffer system and the desired pH; the program then calculates the concentrations of the acid/base species required. In the event the resulting solution does not have the desired pH, The pK Adjuster program is then used to calculate a new pK value for the buffer from the actual conditions. This new pK value is then entered into The Buffers Table. The Solution Formulator program is then used to change the original recipe. This method of calculating the chemical composition of buffer solutions is in error and is not a proper analytical procedure since it does not take into consideration the ionic strength of the solutions. The pK Adjuster program, however, was designed for the determination of the acid/base species required for buffered systems used in the Life Sciences that can contain thousands of undefined components and the ionic strength of which cannot be determined. The Acid–Base Program for Chemistry is dedicated to acid–base systems. This program has a number of options available when calculating acid–base systems: (1) the chemist can choose the weak acid–base system, the concentrations, the pH, and the ionic strength and the program calculates the quantity of strong acid or base required; (2) for low or high pH buffers, the program will calculate the amount of strong acid or base required based on the desired concentrations and ionic strength; and (3) for a given pH, the program will search for suitable substances. In addition to acid–base calculations this program can calculate α values and then plot the α values, log α, or log concentration as a function of pH. It will also plot titration curves for both strong and weak acid–base systems.

LabSolutions, however, carries out calculations not available in The Acid–Base Program For Chemistry. The software will calculate all types of chemical formulations, determine linear and geometric dilution procedures, and determine molecular weights from either formulas or common names.

LabSolutions carries out calculations that can be performed on a hand-held calculator. However, with the storage of chemical data and previously calculated chemical formulations, it will save the bench chemist time and eliminate errors when carrying out quick calculations and looking up chemical data.

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University of North Carolina

PlotView. Version 2.2. Stevens Creek Software: 21346 Rumford Dr., Cupertino, CA 9501. List Price $99.95; mini-site license $279.95; full-site license $579.95. No discounts mentioned. Not copy protected.

PlotView is a Hewlett Packard plotter emulation package for the Apple Macintosh family of computers. The only hardware required is a cable ("Mac to modem" type) and a gender changer to connect the Mac's RS-232 port to the input cable that normally connects the host computer and the plotter. In order to output from the Mac to an HP plotter, a null modem connector is also needed. The software has five operating modes. The first allows the user to capture the data stream of HP graphics language (HP-GL) commands normally sent to create a plot of the data, interpret them, and display the plot on the Mac screen. The second mode is used to read and interpret an existing file of HP-GL commands and display the corresponding screen image. The third mode permits HP-GL commands to be input directly from the keyboard. These are immediately interpreted and presented in graphical form on the screen. This mode might be useful for those wishing to learn HP-GL commands or to software developers. The fourth mode permits exporting a file of stored HP-GL commands to a compatible plotter. When none of these are invoked, the program operates by default in the fifth mode, which continuously listens to the incoming data stream via the open modem connection, and allows the stream to be displayed as text and captured in a file without interpretation as screen graphics. This is useful for rapid (9600 baud) data acquisition and verifying proper communications. PlotView also works with systems that require two-way communication with the HP plotter for various purposes, such as reporting error status, etc. The incoming data stream can be displayed in a separate window and captured if so desired in all operating modes. An abort function is also available that allows immediate termination of input or output in any mode at any time. Besides the obvious uses, this can be used to terminate incoming plots that do not terminate themselves, principally those that do not finish with a "page" command. Graphic images are stored as PICT files, which are object oriented rather than bit mapped. This permits efficient editing of axis labels, baseline smoothing, etc. with programs such as Super Paint operating with the draw layer.

Since HP plotters and Macintosh computers are quite different in the ways they process and present data, some discussion of PlotView's input stream interpretation is appropriate. PlotView does not interpret all HP-GL commands. The authors have chosen 26 as the major ones in use for scientific plotting. Others are simply ignored, and so the final image may differ from that expected. Many commands are executed differently depending on menu choices made within PlotView, such as paper size or pen color. Three menus are provided to deal with paper, pen, and font options, respectively. For example, a monochrome Mac SE can be used to collect the data at the instrument, as this reviewer did, and the remote computer output that was originally formatted for an 8-color HP7440A plotter was displayed as either black or gray lines with PlotView's two color pen option. The data file was later transferred to a Mac II, where the original eight colors could be displayed on the screen. The font menu requires some experimentation for each instrument/computer combination. As the default, PlotView adjusts the font size and type as requested by the remote computer which sends it the data stream. This often leads to very small type sizes, for example, 5 point Courier, which must be edited later. If larger font sizes are forced during data acquisition, this may lead to overlapped lines or crowded print strings. Each different plotter type and application will require specialized treatment. The issue is further complicated when preparing printer output by the fact that HP plotters use a monospaced sans-serif font. These are not normally found on the Imagewriter (except for Monaco) or the LaserWriter. Often one can get sans-serif (such as Helvetica) or monospaced fonts (such as Courier), but not both, usually. So, PlotView uses Courier if it is installed and gives options to also use Monaco and Helvetica. Otherwise, it uses only Monaco.

Two other menus are available, one for communications and one for graphics manipulation. Graphics can be saved to the clipboard or printed to the Mac's printer, and also resized to 75% or 50% of the original. The communications menu has a standard choice, which offers the settings commonly used with HP plotters and also a set-up menu of choices for changing these within the usual range for baud rate, parity, stop bits, and data bits. As a test of the start-up menu, connection was made to an IBM xy plotter with the appropriate menu settings. The software had no difficulty capturing the data stream, although subsequent editing was

necessary to convert the commands to the HP-GL format. The incoming data stream is displayed in a two line, full screen width window at the top of the screen. End of line characters are displayed in reverse video. The above information is clearly described in a 32-page user guide that comes with the software disk.

The data collection features of the software were tested with the Mac SE with a 20 mb internal hard disk, with the Mac II in an Appleshare network, and also with VAX and Prime computers with either Kermit or Chemtalk communications protocols. A Nicolet FTIR system (HP7440A plotter) was used to provide instrumental data, and a molecular modeling package from Molecular Design Laboratories provided test data from the mainframe computers with HP7550A, ColorPro, and 7570A plotters. Several programs were used to edit the PICT and text files produced by PlotView, including Microsoft Word v.4.0, Wingz, MacWrite 11, Super Paint 2.0, and MacDraw v.1.9.5.

Several trials were made in which the data were simply captured in a file by Plot View and then exported directly to the plotter. In all instances, data input and output to a plotter was easy to set up and gave results that were virtually indistinguishable from the original, except for those cases that involved HP-GL commands not interpretable by Plot-View. The data collection process using the Mac SE worked best in the simple listen mode without simultaneous plotting, as recommended in the accompanying manual. If the incoming data were captured and plotted simultaneously, occasionally and randomly a command was garbled, which generally led to extra or missing lines. No such problem appeared during output from PlotView running on either the SE or the Mac II to the plotter, and clean files of correct HP-GL commands always produced good plots. Text files containing HP-GL commands were read and interpreted cleanly to the screen display, although the difference between the speed of the Mac II and the SE is quite apparent for large files. The program communicates with external devices solely through the RS-232 port. PlotView runs cleanly in the Mac II using Multifinder with Super Paint or Wingz. Although the manual cautions that it is possible to encounter limitations with large files, we had no problems manipulating data files for FTIR, NMR, capillary GC, or space-filling representations of 30-atom molecules with shading.

PICT file modification was done with Super Paint and MacDraw, although other software that reads PICT files should work equally well, such as PageMaker or Ready,Set,Go!. A call to Stevens Creek Software (408-725-0424) should clarify any questions. Since each element of the plot is an object, one can easily clean up plot features including data, titles, grid lines, legends, shading, etc. in order to produce high-quality graphics for LaserWriter output. This is very useful for producing text information on the plot in the same font as is used in the document narrative. Then, by using the Mac's Clipboard and Scrapbook features, plots can be pasted into documents.

The text files were readable with Word, Wingz, or MacWrite. If the user is conversant with the HP-GL language, the text files can be altered to produce the desired plot features. There are some good uses for the text files. They can be captured during the experiment on disk for later use, perhaps by a high-quality plotter in a graphics production facility, or modified to emphasize desired features, add a logo, change pen colors or paper sizes, etc. Another use is to put all incoming files from various instruments or software packages in the same format for report production or archival purposes.

The price structure is unusual in that two types of site licenses are available. The mini site license is intended for a limited number of users, such as for a department, and the full site license covers all users at a site. Site licenses include updates and other support.

In summary, PlotView is a very useful general emulation program for acquiring, saving, and using HP graphics information in a Macintosh environment. It is straightforward to learn and use and produces standard output that can be read by other software for the Mac or any HP plotter. It can handle large files with many vectors such as are found in molecular models of enzyme/substrate interactions or CAD graphics and would be useful in almost any application involving HP plotters.

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Dynamical Software I.4 and II.2 are unimaginatively named packages of FORTRAN programs designed for the investigation of nonlinear dynamics and chaos. They operate in MS-DOS environments (PC, XT or AT, or PS-2). Together, they constitute an extensive and sophisticated set of tools for building models and investigating their dynamical properties.

I.4 and II.2 are not likely to be of interest to dilettantes. These packages are formidable in sheer volume, and they also demand significant personal computer resources. I.4, I.4.1, and an enhancement called "SCANNER" arrive on sixteen 360 KB floppy diskettes. II.2 comes on eleven additional floppies. The Demonstration program is distributed on one, 1.2 MB diskette. The software is not copy-protected. The package occupies about 2 MB of disk space, but you need another 1.5 MB for a FORTRAN compiler and more for your own workspace. It is claimed to be possible to run the programs on a floppy-only system, but it would be *extremely* inconvenient to do so, and 1 did not try it. You must have a little over 580 KB of available RAM on whatever computer you are going to use, which means that you need 640 KB total, and virtually no RAM-resident programs other than DOS.

If you wish to investigate the dynamics of your own differential equations, it is also necessary to have available a fairly recent FORTRAN compiler. Microsoft 3 or 4 are recommended, although a patch that allows use of Ryan-McFarland 2.11 or later is also available on request from the vendor. One can also utilize the powerful analytical capabilities of the package to evaluate either experimental data or dynamics generated on another computer. In this case, a local compiler is not needed. A coprocessor is not required, but it is highly recommended for the intensive floating-point operations that the software is designed to do. The package supports mouse usage, but it does not require it. It includes a clever mouse-emulator that utilizes the keyboard arrow keys and "insert" and "delete" for the mouse buttons and was found to be a workable alternative. I was able to run the system (slowly) on my AT-clone, but most of the testing for this review was accomplished on a borrowed 80386 machine with 80387 coprocessor, running Microsoft FORTRAN 4.1 under DOS 4.01. Graphics are among the most important features of the package. The software requires Hercules, CGA, EGA, or Vega Video Deluxe graphics.

Documentation for the software is extensive and accurate. The User's Manual for I.4 runs 194 pages, of which the first chapter is an introduction to chaos and strange attractors. The rest consists of instructions for loading and using the software. I.4.1 is accompanied by its own short volume. II.2 has an additional 239-page manual. The documentation includes numerous examples showing the appearance of screens as various commands are entered and executed. There is also an on-screen "manual" that reminds one of the syntax for the commands of the Dynamical Systems software.

If the developers were short of imagination when it came to names, they certainly were not when it can to writing useful software. Most of the techniques of interest to an investigator of nonlinear systems can be found in 1 or 11. I.4 provides the essentials: an Adams-type integrator, a map driver, and facilities for two- or three-dimensional plotting, and the ability to plot discrete maps from continuous data. Four kinds of mathematical models are pre-programmed, and random noise can be added, if desired. With the SCANNER subroutines, differential equations are programmed directly from their algebraic representation, greatly simplifying the generation of new models. II.2 includes a Runge-Kutta integrator, integration of delay differential equations, two-dimensional phase portraits for different initial conditions, bifurcation and rotation diagrams for discrete maps, spectral analysis, estimation of fractal dimensions and Lyapunov exponents for time series, and additional graphics capabilities. The best feature of these packages is that they are all very accessible to the investigator. Everything is written in standard FORTRAN code and can be altered to fit the needs of the user. The chemist interested in a system characterized by a system of coupled differential equations, such as oscillating chemical reactions, will find that this package will save several months of work by a skilled programmer and will produce better-quality results than most scientist-programmers would write.

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