Additions and Corrections

Acylation of β-Lactams by Class A β-Lactamase: An *ab Initio* Theoretical Study on the Effects of the Oxy-Anion Hole [*J. Am. Chem. Soc.* **1997**, *119*, 6423−6431]. BRIAN D. WLADKOWSKI,* SARAH A. CHENOWETH, JULIE N. SANDERS, MORRIS KRAUSS, AND WALTER J. STEVENS*

In Figures 3 through 7, as well as various locations in the associated text, Gln-245 is incorrectly labeled. The residue should be referred to as Gln-237 throughout.

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Computer Software Reviews

IGOR Pro, Version 3 (Mac). Wavemetrics, Inc.: P.O. Box 2088, Lake Oswego, Oregon, 97035. Phone: (503) 620-3001. Fax: (503) 620-6754. E-mail: sales@wavemetrics.com, http://www.wavemetrics.com. List Price $495.00; students and faculty $346.50; additional quantity, multi-user, and coursework discounts available.

IGOR Pro is an extremely powerful data analysis and graphing program. IGOR Pro 3.03 is the current shipping version, which requires system 7.0 or later. The IGOR installer includes versions of the program for 68K Macs with or without a floating point unit, as well as a PowerMac-native version.

Although Igor can handle data in a variety of forms, its strength is manipulating waveform data, such as that collected from spectrometers and other scientific instruments. This sort of data typically consists of thousands of values measured at evenly spaced intervals. Igor's basic data object is a "wave", in which the *y* component of each data point is stored explicitly, while the *x* component is calculated based on the wave's "X scaling" factor. Igor handles data which do not fit the waveform pattern ("XY data") by treating two waves as an XY pair, in which one supplies the *x* values while the other supplies the *y* values. The user can input data directly, or import data in various file formats, including tabdelimited text.

Igor can deal with data sets of unlimited size, with up to four dimensions per wave (not including the X scaling). There is no limit to the number of data sets contained in one experiment. The analysis tools available for waveform data include multi-dimensional fast Fourier transforms, integration and differentiation, and smoothing, with choice of algorithm. On both XY and waveform data, Igor can do curve-fitting to standard functions or to any user-defined fitting function, as well as statistical analysis, peak and level detection, and calculation of area under a curve.

Igor's graphics capabilities are equally powerful and flexible. The number of curves and axes on a graph is unlimited, and the user has complete control of every aspect of the graph. The program can also create image and contour plots, and has some image-processing capabilities. Wireframe and surface plots are not available, but may be included in a future version. Igor can export graphics as PICT or EPS files.

The program comes with many extensions, to do such tasks as transferring data via the sound input and output ports, the loading MATLAB, Nicolet, or GW Instruments files. In addition, users who purchase the optional External Operations Toolkit can create their own extensions by programming in C. Some waveform and surface plot types have been added in IGOR Pro 3.03. Updates from earlier versions are available from:

<ftp:/ /d31rz0.stanford.edu/WaveMetrics/IgorPro/FilesUpdate/>

The most impressive aspect of Igor Pro is its flexibility. All parts of the program can be altered by the user, including dialog boxes, menus, and help files. Igor comes with a built-in programming language and extensive help to allow users to create their own procedures or change existing ones. Taking advantage of the flexibility and power does require some effort on the part of the user: a new user can sit down and learn how to make graphs from data tables relatively quickly, but will be confused by many aspects of Igor until going through the "guided tour" manual provided. This tour takes about 2.5 h to complete, and gives a good overview of Igor's capabilities and of "waves". In addition, the program comes with a 750+-page User's Guide, a 450-page Programming and Reference Manual, and on-line help files, all of which are very informative and easy to use.

Igor Pro is a sophisticated data analysis package, which will be especially useful for heavy-duty applications such as analyzing lab spectra. The manufacturers have taken great care to make Igor accessible, and allow the user to take full advantage of the program to do whatever the *user* wants it to do.

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Grapher for Windows Version 1.30 . Golden Software, Inc.: 809 14th Street, Golden, CO 80401-1866. (800) 972-1021; (303) 279-1021. List price $199.

The majority of graphing programs on the market let a user select a graph type from a long list. This list usually contains graph types that, beyond some small differences, e.g., presence or absence of grids, are virtually the same. The approach taken by the Grapher creators is different. Only four graph types are listed in the graph menu, e.g., line or symbol, bar chart, high-low-close, and function. Also included is a template for a ternary graph. However, each graph type can be easily customized, which makes Grapher a versatile graphing tool. Three different axes, namely linear, logarithmic, and probability, are available and any combination of them can be used. The axes with both ascending and descending data values can be displayed and positioned at any location including, for instance, a case of two axes crossing in the middle. Grapher lets a user display an unlimited number of axes, but a data set is always associated with one X and one Y axis. Therefore a user cannot create a graph with two active Y axes for two different quantities plotted. This problem may be solved, however, by recalculating data, if necessary, and creating an additional axis labeled with desired units. Alternatively, a set of two or more stacked graphs can be created. The axes can be labeled with either numbers (in a variety of formats) as well as with date or user defined text labels. Data point labels and grids can also be displayed on a graph. It is also possible to create horizontal and vertical error bars in which length is either automatically calculated or user specified. An additional option for bar charts is a choice between stacked, adjacent, or partially overlapping bars. The user may also specify the Y value from which the bars originate. Function plots can be defined by either a simple $y = f(x)$ equation or by a set of parametric equations $x = f(t)$; $y = g(t)$. The library of mathematical functions includes some less frequently used but important functions like Bessel functions or random number generators.

The following fit methods are available: linear, linear through origin, exponential, power, polynomial (degree 0−10), running average, and spline smoothing with different tension factors. The lack of a user

defined curve fitting seems quite surprising and is the most serious shortcoming of the software. The method of selecting the data to be plotted (fitted) could also be improved. Unlike other programs (for instance DeltaGraph or KaleidaGraph) the Grapher offers only an automatic selection of either data limits or data interval at which data are plotted. The temporary removal of some randomly distributed data points can only be done by cutting the data and pasting them to some other location in the worksheet. Such a procedure is not only time consuming but also may be confusing and result in loss of data. The graph, i.e., plots and fits are automatically updated after any change of data file.

A virtue of the program is its speed, a factor important to users having relatively slower computers and/or plotting large data files, especially those generated as output of some measuring devices. Creating a plot showing five voltammograms, each represented by an ASCII file containing 1000−2000 potential-current pairs, took just a few minutes. The same task could be accomplished in incomparably longer time when DeltaGraph Professional 3.5 was used. In both cases there was no extensive use of a Windows swap file. In the newer, 4.0 version of DeltaGraph, however, the speed of the program is said to be significantly improved. The good performance of Grapher is not only due to the speed at which graphs are plotted but also to the way in which elements of the graph are handled. Any element of the graph, e.g., axis, plot, experimental points, bars, fit line, graphics, and text, may be easily selected with a mouse. Double clicking on the mouse brings an immediately corresponding dialog box that lets a user specify desired modifications, which are then promptly executed.

Any completed graph may be used as a template to create several closely related graphs. When only a hard copy is needed, a template graph may be used to print automatically graphs of several closely related data files. However, automatic printing of a number of existing graphs at one time is also possible. Exporting graphs to another Windows application is performed through a clipboard. Depending on the application, the graph is pasted as either a bitmapped image or a picture (Windows metafile). Graphics in the above two formats as well as text can be imported into Grapher and placed on a graph. The worksheet, on the other hand, accepts files in ASCII, SYLK (.SLK), EXCEL (.XLS), and Lotus (.WK1 or .WKS) formats. In addition, many files can be merged into a single worksheet.

Grapher offers simple drawing tools (polygon, line, rectangle, rounded rectangle, ellipse, or circle) as well as a math text editor. The editor lets a user place mathematical expressions on a graph. It is also useful when an axis has to be labeled with Greek or mixed Greek and Roman characters. Unfortunately, use of the editor is not easy, because it requires a knowledge of the special syntax.

Data and graphs created by the Grapher are stored in separate files. This helps to reduce hard disk space usage, but may create a risk of accidentally deleting a data file, since, beyond the user defined file names, there is no indication of a link between graph and data files.

In general, Grapher is easy to use due to the widely applied intuitive point and click method. Some operations, however, require applying procedures that are not intuitive. A perfect example, besides the math text editor, is creating tick labels in exponential format. To do this, the user has to import a special file into the worksheet. Fortunately, the Grapher manual is written well.

In summary, Grapher can be recommended for users who routinely plot large data files and do not need to perform advanced curve fitting. Others may find other programs more useful.

Grapher comes on two 3.5 in. HD disks. A user can make a single copy of the installation disks for backup purposes. The program takes approximately 2.5 megabytes of a hard disk space. A computer running Windows 3.1 or later with at least 4 megabytes of memory is a minimal system requirement to run Grapher 1.30.

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Book Reviews

Studies in Surface Science and Catalysis, #103: Semiconductor Nanoclusters—Physical, Chemical, and Catalytic Aspects. Edited by P. V. Kamat (University of Notre Dame) and D. Meisel (Argonne National Laboratory). Elsevier: Amsterdam, 1997. x + 474 pp. $272.00. ISBN 0-444-82064-7.

In recent years there has been a dramatic increase in research on nanoclusters and nanocrystalline materials. This interest has cut across the traditional boundaries of chemistry, physics, and engineering. The interest in semiconductor nanoclusters is largely due to the phenomenon on quantum confinement, whereby the optical and chemical properties of the nanocluster are size dependent. Quantum confinement is typically observed in particles with diameters less that 10 nm, which defines the size of most of the nanocluster systems discussed in this text. The chapters in this book cover a broad range of topics and are well referenced. In particular, the focus is the chemical behavior of semiconductor nanoclusters and nanocrystalline semiconductor electrodes. It very successfully brings together aspects of nanocluster spectroscopy and photophysics and many applications of the nanoclusters and nanocrystalline electrodes. This text is aimed at the graduate student or research scientist wishing to gain familiarity with what has become a rapidly expanding field.

The book starts out with chapters on the basics of semiconductor nanoclusters: synthesis and characterization of nanoclusters and their mechanical and surface properties. This provides a foundation for many of the following chapters. There is also a chapter covering both the theory and current literature of electron transfer at nanocluster interfaces. This is of great importance because many, if not most, potential applications of semiconductor nanoclusters involve interfacial electron transfer. Along the same lines, there is a chapter on composite semiconductor nanoclusters. This chapter focuses on TiO_2/SnO_2 and TiO_2/CdS systems. Charge transfer, resulting in electron/hole separation, is very efficient in these systems, making them potentially useful photocatalysts.

Luminescent porous silicon has been a subject of intense interest in recent years. There is a chapter which reviews the synthesis, chemistry, and applications of this material. The emphasis of the chapter is on the mechanism of luminescence and how the luminescence properties are modified by the surface chemistry. There is also a chapter on the theory of quantum-confined silicon particles.

Nanocrystalline semiconductor electrodes are currently of very great interest. Much of this interest has been stimulated by the development of efficient, dye-sensitized injection solar cells. Specifically, ruthenium(II) tris(bipyridine) and similar molecules have been used to sensitize nanocrystalline TiO_2, resulting in remarkably efficient solar cells. The principles of operation of such solar cells are reviewed in a chapter of the book. The chapter also discusses their long-term stability, which is of great practical importance.

The final chapters of the book discuss the use of nanocrystalline TiO_2 to catalytically photo-oxidize organic molecules. This oxidation may occur through several different mechanisms. Photoexcitation of TiO_2 produces surface-trapped electron/hole pairs. Oxidation may proceed directly form the holes, or both holes and electrons (in the presence of O_2) may produce hydroxyl radicals. The use of technologies based on these reactions are sure to expand, as our need to remediate hazardous waste grows.

Topics other than those mentioned above are also discussed in the book, making it an excellent overview of the field. There is, however, one big problem with the book—the price. At $272.00 it cannot be used as a text in a special topics course, for which it would otherwise be well suited.

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