Computer Software Reviews

KaleidaGraph 3.0.5 for MacIntosh and Windows. Synergy Software, 2457 Perkiomen Avenue, Reading, Pennsylvania 19606-9976. Phone: (610) 370-0548. Fax: (610) 370-0548. E-mail: maxwell@sales.synergy.com. $249.00.

KaleidaGraph is a graphing and data analysis software package for the Macintosh. It is also available for Windows 95, Windows NT, Windows for Workgroups 3.11, and Windows for Workgroups 3.1.

KaleidaGraph is installed using an installer. Floating point unit and Power Macintosh versions are included, although the software will run on more modest machines. The manufacturer claims any Macintosh with 2Mb RAM, a hard disk, and System 6.0.5 or later is capable of running Kaleidagraph. A reference guide and a tutorial manual are provided.

KaleidaGraph has a simple and uncluttered interface, which makes it easy to learn. This apparent simplicity hides very powerful tools, however. Using KaleidaGraph, it is possible to make graphs that are not possible in spreadsheet programs because of the vast amount of data points involved. KaleidaGraph also has a built-in macro programming language and support for Apple Events which enable the user to customize KaleidaGraph. Thus, it is possible to graph and analyze data from a variety of sources. KaleidaGraph contains a macro calculator which is used to make and test macros and to perform general calculations on scalars. The programming language used in KaleidaGraph is assembler (machine language) like, which makes it rather hard to learn and understand if one has not been exposed to BASIC or assembler previously. Another curiosity is that the macro calculator is a RPN or stack calculator à la the old Hewlett-Packard calculators. Presumably this aids in the execution of calculations, but it does tend to make using the calculator a chore if one is not used to using a stack calculator.

In addition to the simplicity of performing most of the tasks, the most impressive thing about KaleidaGraph is its speed. For example, a plot of a data file containing 32 000 elements took barely noticeable time on a PowerPC-based machine. Likewise the curve-fitting functions are extremely fast. The most nonintuitive operation in KaleidaGraph is the use of templates. With most other programs one first creates the template and then places the contents into the template. In KaleidaGraph a template is created by first making a plot and arranging the titles, legends, etc. until the desired form is achieved. After this the plot is simply declared a template and is used by changing the data. The templates also remember the axis ranges, thus making it easy to compare different data sets and plots.

KaleidaGraph allows exporting of data in binary and text form in addition to the normal KaleidaGraph format. Plots can be exported in either PICT or MacPaint form. It is also possible to export plots in EPS form, if a LaserWriter 8 printer driver is installed. Choosing "Print to file" in the printing dialog box, one can save the graph as an EPS file for importing into a graphics, text processing, or page layout program. This is a very nice feature as the EPS file can be imported to Adobe Illustrator 6.0 as parsed EPS where each data segment is represented in the graph as an individual line. These objects can be edited individually or as a group for custom, high-quality output.

All in all, KaleidaGraph is a well-made and stable program for doing graphing and data analysis. Its major advantages are speed, small size, and capacity to handle large amounts of data points. In addition the product is attractively priced. On the con side, the macro calculator and macro language are awkward to use and may be intimidating to many people. Fortunately, it is not necessary for most people to use the macro facilities, because the most common operations can be done without scripting.

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Book Reviews *

Catalytic RNA. Series: Nucleic Acids and Molecular Biology, #10. Edited by Fritz Eckstein (Max-Planck-Institut) and David M. J. Lilley (University of Dundee). Springer: New York. 1996. xi + 417 pp. $197.00. ISBN 3-540-60795-1.

The book consists of 22 chapters written by various authors on different aspects of the title topic. Each of the chapters is 10−30 pages long and serves as a review of a particular aspect of the catalytic RNA world. Most of the book is written so that little previous knowledge of RNA catalysis and structure is required to follow the text, making it suitable for newcomers to the catalytic RNA field, and in addition, it adequately fills the needs of the advanced RNA scientists by providing a convenient source for the various ribozyme systems covered. Each chapter includes a thorough list of references for the reader if he/she wishes to find more details on the methods and/or results discussed within the chapter. This book is, for the most part, well organized and well written. Numerous spelling errors do, however, detract from the otherwise high quality of writing.

The first three chapters discuss the group I intron, the first self-splicing RNA discovered. The first chapter gives an excellent overview of group I intron kinetics as well as discusses key tertiary interactions for catalysis. It also discusses some proposed interactions which take place immediately prior to the cleavage event. The second chapter also looks at the group I intron from a kinetic point of view, using fluorescent probes to determine rate constants for the individual steps of trans-substrate base pairing as well as formation of the fully docked complex. The third chapter presents the Michel−Westhof model of the tertiary structure of the catalytic core of the group I intron and discusses some aspects of the model in more detail. In the six years since its initial proposal, this model has held up quite well.

One chapter each is dedicated to biochemical studies of the hairpin ribozyme, Rnase P RNA, and group II intron. While the limited space afforded each of these categories of RNA prevents any extensive coverage of each field, informative summaries of current and past research are provided for each.

Four chapters address the hammerhead ribozyme mechanism. While there is a substantial degree of overlap with regard to the information presented in each of these chapters, the various methods of study employed to obtain the information (crystal structures, fluorescence resonance energy transfer [FRET] measurements, cross-linking, mutagenesis, base analog substitutions, as well as traditional biochemical methods of analysis) add to the confidence of the consensus structure and the mechanism of catalysis.

Approximately one-third of the book is dedicated to ribozyme-based gene therapy. Various topics like ribozyme delivery methods, functional group modifications for increased RNA stability, and results from *in vivo* studies with endogenously expressed ribozymes are covered. Three of the chapters are dedicated specifically to anti-HIV-1 ribozymes. In these chapters, ribozyme delivery schemes, ribozyme/target colocalization, and target selection rationale are addressed. Each of these aspects must be addressed for any ribozyme-mediated therapy to be successful.

The last two chapters discuss *in vitro* selection of RNA structures. This method has been used to obtain RNA structures which support

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unusual catalytic activities as well as to define structure/function relationships with RNA. It represents a valuable addition to the book.

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Surface Analysis with STM and AFM: Experimental and Theoretical Aspects of Image Analysis. By Sergei N. Magonov (Digital Instruments, Inc.) and Myung-Hwan Whangbo (North Carolina State University). VCH: New York. 1996. xii + 323 pp. $125.00. ISBN 3-527-29313-2.

The importance of the scanning tunneling microscope (STM), the atomic force microscope (AFM), and other related instrumentation (known collectively as scanning probe microscopes) for the examination and characterization of surfaces and interfaces is by now well established. Virtually no aspect of interfacial science remains untouched by these microscopies, and there is hardly a laboratory concerned with these subjects without access to one or more of these versatile instruments. The proliferation of probe microscopes has led to a corresponding proliferation of review articles and books which examine all aspects of scanning probe microscopes. *Surface Analysis with STM and AFM* by S. N. Magonov and M.-H. Whangbo is a welcome addition to this literature.

The authors summarize in the introduction that the book is "primarily concerned with how the surfaces of various materials are characterized by employing STM and AFM, and what physical/chemical features can be deduced from their images". The focus of the book is primarily directed toward understanding STM and AFM imaging in the ambient environment, and the choice of examples—and computational methods—reflects this emphasis.

The book is divided into three sections. In the first, introductory section, the authors discuss the background and fundamentals of probe microscopy. The first chapter discusses some key problems in STM and AFM applications including tip—sample interactions, surface relaxation and local hardness, and surface forces in AFM. The second chapter describes physical processes relevant to AFM and STM, and the third discusses the main components of the instrumentation along with AFM and STM operating principles. A fourth chapter on practical and experimental aspects of AFM and STM imaging will be especially helpful for the beginner.

In the book's second section, the authors provide the information necessary to understand their simulations of STM and AFM images, including background on the electronic structure of solids, some models of the tunneling process relevant to STM, and background on AFM. The electronic structural material is necessarily sketchy, but brings together important concepts with references for more involved study.

Finally, the third and longest section of the book describes STM and AFM images and associated analysis of several systems. These systems include layered inorganic compounds, point defects in layered compounds, organic conducting salts, alkanes layers on HOPG and β-Nb_3I_8, self-organized amphiphiles, and polymer materials both as crystals themselves and as films on surfaces. A major theme of this section is the importance of tip—sample interactions in inducing defects and deformations in the sample under study and the way in which these deformations influence the appearance of the STM or AFM image.

The book's greatest strength is the authors thorough review of work on the electronic structure of layered surfaces and related systems. For investigators of these materials, and for anyone imaging in the ambient environment, this book will be an invaluable reference. The introductory sections—especially those describing artifacts—are very appropriate for all users. This is also the first book to explicitly review in detail the connection between the electronic structure of solids and the STM image, and it provides a firm introduction to this important topic.

This book's greatest weakness is its somewhat parochial point of view. There is almost no mention of studies on surfaces not in the ambient air environment. This is an unfortunate oversight, because the most important scientific contributions of the STM and AFM technologies have come from work in UHV, in the electrochemical environment, and in other controlled atmospheres. Also, because of its focus on work in ambient environments, the authors overemphasize the role of the tip—sample interaction in deforming the sample. This interaction is important everywhere, but does not have the same overwhelming influence in environments where the contamination layer—inevitable in studies in ambient—is not present. Finally, the authors' electronic structural analysis also reflects a narrow point of view. The authors do not review work studying more strongly chemisorbed adsorbates, or other important advances in calculating STM images. This oversight undoubtedly drives from the particular focus on ambient imaging—where chemisorbtion is hard to control and consequently less well studied.

There are a number of other texts that provide a more well-rounded overview of STM and AFM. A good general flavor of the field—although now already somewhat dated—can be had from the Springer-Verlag series *Scanning Tunneling Microscopy I, II, and III*. Nonetheless, *Surface Analysis with STM and AFM*, with the caveat of its somewhat restricted focus, is an important addition to the literature.

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4th World Surfactants Congress, Volumes 1−4. The Royal Society of Chemistry: Cambridge. 1996. 1920 pp. £159.50. ISBN 0-85404-751-4, 0-85404-756-5, 0-85404-761-1, 0-85404-766-2.

This series of four books brings together the lectures and posters presented at the 4th World Surfactants Congress, which took place in Barcelona, Spain, June 3−7, 1996. The four volume titles are (Volume 1) Economic Outlook, Raw Materials, Synthesis and Characterization, (Volume 2) Properties and Applications, (Volume 3) Toxicology and Environment, and (Volume 4) Posters from all the previous selections. This book represents a distillation of the work of the current specialists in surfactants technology. The specialists examine the current state-of-the-art technology, the market for surfactants, and the raw materials available. This series of books offers the latest available information on the state of the surfactants world today, and it will be essential reading for those in academia and industry who need to keep abreast of technological, economic, and environmental considerations.

Gmelin Handbook of Inorganic and Organometallic Chemistry. Supplement Volume C1: Mononuclear Compounds with Hydrogen. Edited by Dieter Koschel and Hans Schafer. Springer: Berlin. 1993. xvi + 326 pp. ISBN 3-540-93680-7.

This volume C1 is the first supplement volume to *Phosphor C* which was published in 1965 and covers the compounds of phosphorus. Starting with the binary species formed between phosphorus and hydrogen, the present volume deals with the neutral mononuclear compounds PH through PH_5; the ions featuring the same stoichiometric composition are covered in separate sections. The first two chapters cover PH and PH_2, their physical and mostly molecular properties. The critical coverage of the large number of papers considered to be relevant for the description of PH_3 amounts to about 197 pages. The last chapters, in addition to other ionic species, deal with the description of PH_4. There is a chapter on physical constants and conversion factors.