Computer Software Reviews

PSI-Plot Version 4.52 for Windows/Windows 95. Poly Software International, P.O. Box 526368, Salt Lake City, UT 84152. Phone: (801) 485-0486. List price $299.00.

PSI-Plot is intended as a general purpose technical plotting and data processing program, with the ability to produce two- and three-dimensional plots of publication quality. It includes implementations of several methods for the numerical solution of ordinary differential equations, as well as a variety of speciality plots, such as ternary (triangle) plots, Smith plots, polar plots, quality control charts, etc., and a reasonably complete set of statistical routines for data analysis, including user-defined as well as prepackaged functions for curve fitting. It also features the ability to generate and plot complex parametric two- and three-dimensional curves and surfaces. It requires an IBM PC or compatible with an 80 × 86 or Pentium processor running Windows 3.1 or Windows 95, 2 Mbyte or more of memory, and 4 Mbyte of free disk space. The program is not copy-protected.

The choice of a plotting package is a highly individual one, and most such packages have their share of major and minor bugs and quirks. If the program is sufficiently flexible and convenient, the user learns to coexist with these, and hopes for a newer version in which at least some of them have been removed. There is an inevitable reluctance to learn to deal with the corresponding quirks of a new piece of software, particularly if the user is interested in the final plot and not in the process of making it. PSI-Plot has enough features and promises enough power to make overcoming this reluctance seem attractive. Unfortunately, in the opinion of this reviewer, the program has some major design flaws and a very large number of very serious bugs. These problems make the program very much less useful than it should be.

Making a simple *XY* plot using this program is reasonably simple. A spreadsheet-like page (called the "sheet") containing the data is first constructed, and then a plotting page (called the "plot") is opened. The type of plot desired is chosen (from a long submenu of options), and a dialog is opened which includes a list of column titles from the sheet, together with several style and color choice subdialogs. The appropriate columns are indicated by clicking on their names and assigning them to the *X* and *Y* axes of the plot (for more complex plot types, the dialog box is modified appropriately and relatively transparently). Since the data sheet is not visible while this choice is being made, the user would be wise to give the columns descriptive names; in a sheet with many data columns it would be quite easy to get lost otherwise. Once the choice of *X* and *Y* data is made, the "Add Curve" is clicked, and more pairs of columns can be selected similarly. No visible feedback is available about which columns have been chosen, beyond a count of the number of curves on the plot. When all of the desired choices have been made, the "OK" button is clicked, and the plot appears. For each curve, a variety of line and symbol sizes, types, and colors can be used, or the default values accepted. All of these can be modified later by clicking on the desired feature on the plot, though sometimes a bit of effort is required to activate the desired feature (clicking on a small feature of the plot is likely to activate the entire plot rather than just that feature; the user must regularly resort to use of the keyboard to focus the program's attention).

The major problem with PSI-Plot becomes apparent when the plot is saved: the data and the graph are apparently decoupled from one another after the plot is drawn. The plot is saved in one file (with DOS filetype .pgw) while the data sheet is saved in another (with filetype .pdw). The user must save these two files separately; it is possible therefore to inadvertantly save the graph without the data that go with it, and *vice versa*. Further, and even more damaging, changing the data does not automatically change the plot. PSI-Plot is therefore very difficult to use for "what-if" questions, and it is also unnecessarily tedious to correct data entry errors and other changes after the plot is made. The dual-file approach also doubles the bookkeeping problems associated with keeping track of a large number of data sets and plots (it is easy in many applications to generate thousands of plots a year, even for single users). The problems associated with this file structure were aggravated in my copy of the program by a bug: the filed version of the plot was changed from the plotted version, so that when it was recalled, the plot had shrunk to a very small size (just the plot, not the labels and annotations accompanying it). Much of the work of constructing the plot therefore had to be repeated on the recalled version. This bug could be avoided (most of the time) by explicitly sizing the plot before saving.

The plots from PSI-Plot, using the default settings, are barely of publication quality on a good laser printer. It is clear that the power to improve their appearance is in the program, however, so with a little fiddling high-quality output could almost certainly be obtained.

Annotations to the plot are made by choices from a toolbar; it is irritating to me that each click on the toolbar allows only one object to be drawn, so that to create several objects of the same kind (several separate labels, for example), it is necessary to repeatedly click the appropriate button on the toolbar. This is a standard feature of the program. It makes it annoying to experiment with a change in a plot objet (font, color, style, size, etc.), since each time a change is desired, the object in question must be reselected, and this can take several clicks and/or keystrokes. In most cases, changes made to the plot are irreversible; there is no "undo" button on the editor in this mode. In other words, be careful: if an object is deleted, it is gone for good. Simple mathematical expressions can be constructed using a rather awkward script.

Documentation consists of a thick manual that describes most of the functions of the program. It occasionally reads as if it were a word-for-word translation from another language, but is generally adequate. It includes a helpful tutorial, which is indispensible for learning how to use the program.

In spite of these problems, and a number of other less serious, but aggravating, bugs, there are a number of attractive aspects to PSI-Plot. New axes are added logically and easily to an existing graph, and new plots can readily be made on the same page. The output of the statistical features of the program (linear regressions, nonlinear curve fitting, ANOVA, etc.) are unusually complete. For users interested in making certain kinds of specialized plots, such as those mentioned in the first paragraph, or who are interested in the numerical routines PSI-plot offers, this program may be worthwhile. However, for general use, it is my opinion that several other plotting packages are on the market that are much better designed and much less trouble to use.

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JA965930Q

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nQuery Advisor Version 1.0. Statistical Solutions, Ltd., 60 State St., Suite 700, Boston, MA 02109. Phone: (617) 854-7472. Written by Janet D. Elashoff. List Price $475.00.

nQuery Advisor, a software program created to assist in the determination of sample sizes for planning a statistical study, operates with IBM and compatible PCs. Written specifically for Windoes 3.1, it functions with Windows 95 or Windows NT and requires a 386/25 or better processor, 4 Mbyte of RAM and 3 Mbyte of hard disk space. Versions for Macintosh or UNIX operating systems are not available. It is copy protected and does allow for the replication of one copy exclusively for backup purposes. Multiuser and network licenses are obtainable at competitive prices.

Arranged in table format, the software assesses sample size, power or effect size based on means, proportions, survival, agreement and regression, with one, two, or multiple groups using test, confidence interval, and equivalence analyses. Considering equal and unequal sample sizes is possible for most problems. More than 50 types of analyses are available for sample size assessment, ranging from a one-sample *t* test, a univariate one-way repeated measure analysis of variance, a two-sample χ^2 test for equivalence, and a log-rank test for equality of survival curves to multiple linear regression, to name a few.

Given the power, significance level, and effect size, nQuery Advisor computes the sample size through searching for the minimum value required to achieve the specified power. Adopting the reverse approach is possible by proposing various sample sizes and determining the power, effect size, or interval width for confidence intervals. Plots displaying the relationship between power and sample size can be rendered, and tables as well as plots are easily cut and pasted into any word processing document that is compatible with Microsoft Windows.

Computational aids provide assistance in the estimation of standard deviations from standard error, range, percentiles, coefficient of variation, upper confidence limits, and correlation coefficients along with detailed guidance for designing studies based on limited information. For more experienced statisticians who may have an analysis not considered by nQuery Advisor, a distribution function menu is available offering Gaussian, t, χ^2, and F (both central and noncentral for the latter three) distributions where one can insert customized sample size equations.

Installation is swift and simple with all of the files stored on only two diskettes. Detailed documentation clearly describes the icons, sample, and distribution function tables for facilitating choice among a variety of statistical analyses and provides tutorials with sample epidemiological study designs. The software is menu driven with prompts following each selection that guide a less experienced user through the analysis process. Upon selection of an icon, a brief description appears, and guide cards are available that define each cell in an analysis table as well as offer reasonable values for level of significance or power if help is needed for selecting those numbers. It also creates sample size justification statements that explain the sample size decision based on a selected analysis that can easily be edited, cut, and pasted into windows compatible word processing programs including Microsoft Word and Word Perfect for Windows.

Those who plan statistical studies will find this program invaluable for assisting in the challenge of determining the appropriate sample size for a multivariable research study and is probably most useful to those in the field of epidemiology or to researchers who want to avoid wasting resources on too vast a study or a project with a sample not large enough to produce conclusive results. While most other statistical packages including Prism from GraphPad, or Statistica from StatSoft Inc., do not offer the option of determining sample sizes, they do provide more comprehensive statistical analyses. This software package accommodates more extensive interpretation of research data and advises users in selecting a particular statistical analysis after establishing a project. However, in the early stages of project planning one challenge of designing a conclusive statistical study is sample size determination, and that is the novelty and utility offered by nQuery Advisor.

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Book Reviews

Synthetic and Natural Phenols. Studies in Organic Chemistry #52. By J. H. P. Tyman (Brunel University, Uxbridge, U.K.). Elsevier: Amsterdam. 1996. xx + 700 pp. $368.75. ISBN 0-444-88164-6.

In this book the author intends to present an account of developments in phenol chemistry mainly over the last two decades. The author J. H. P. Tyman has published numerous research articles and some special topic reviews on this topic extending over this period of time and is obviously an authority on phenols. Dr. Tyman has succeeded in the goal he has set since most of the references are in the 1980s with a large number in the early 1990s extending to 1995−96 as early as in the first chapter. In addition, much information presented from Tyson's own research is from unpublished work with his students. References are listed at the end of each chapter in order of appearance in the chapter. The oldest (1599) reference in the book—the last in the last paragraph of the last chapter—is to Shakespeare's *Julius Caesar*! Unfortunately the years for granting of numerous patents referenced are not listed (except curiously only in Chapter 1) so that an assessment of their timeliness cannot easily be made. An alphabetical subject index for the entire book appears at the end and a table of abbreviations used appears at the beginning of the book. The emphasis in the book is on synthesis rather than on mechanisms which are briefly discussed in the first chapter. In a dedication, the author reconciles those experimenters in the chemistry of phenolic compounds who have gone before, those of today, and others whose work has escaped mention.

The author has organized the material into chapters mainly on the basis of types of phenols with only two chapters on important reactions—those of hydroxyl groups (Chapter 3) and oxidation (Chapter 5). A listing of the 14 chapters will give readers the overall scope of material covered: (Chapter 1) Historical Aspects and Industrial Syntheses of Monohydric and Dihydric Phenols; (Chapter 2) Recent Advances in the Synthesis of Monohydric Phenols; (Chapter 3) Reactions of the Hydroxyl Group in Monohydric Phenols; (Chapter 4) Phenolic Ethers of Hydroxy Aromatics; (Chapter 5) Oxidation of Phenols; (Chapter 6) Alkyl and Hindered Phenols; (Chapter 7) Carbonyl Derivatives of Phenols; (Chapter 8) Halogeno, Nitro, Amino, Azo, Sulpho and Thio Derivatives of Phenols; (Chapter 9) Dihydric Phenols; (Chapter 10) Polyhydric Phenols; (Chapter 11) Branched Alkylphenols of Industrial Interest; (Chapter 12) Prenylphenols; (Chapter 13) Non-isprenoid Alkylphenols; (Chapter 14) Syntheses of Natural Phenols (and their Derivatives) of Pharmaceutical, Medicinal or Technical Interest.

A few minor criticisms: Although the two-step cumene process for phenol synthesis is discussed in Chapter 1 among other syntheses, a new process based on a one-step catalytic oxidation of benzene by nitrous oxide in which product yield is 99% (compared with 93% for the cumene route) is not mentioned. A plant using this process is being built by Monsanto.

Standard recommended abbreviations are not used for some of the referenced journals and usage is inconsistent in some cases. Thus, although *J. Am. Chem. Soc.* is mainly used, it appears as *J. Amer. Chem. Soc.* occasionally; *Zh. Org. Chim.* (p 89) as well as *Zh. Org. Khim.* (p 331) appear; and *Org. Prep. Proc. Intern.* as well as *Org. Prep. Proc. Int.* Reference 100 (Chapter 11) lists *ibid.*, but the previous reference is a patent! Reference 144 (Chapter 9, Tyman et al.) lists *J. Chem. Soc. Perkin Trans I*, but no year or page is given. In addition to better proof-reading, many of these deficiencies in references could be overcome by adding an alphabetical author index.

In conclusion, since the book will be a reference source for phenols for some time, it is recommended for libraries; those doing research extensively in this area may also wish to invest in a copy for ready reference.

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JA9755065

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Early Transition Metal Clusters with Pi-Donor Ligands. Edited by Malcolm H. Chisholm (Indiana University). VCH: New York. 1995. xii + 289 pp. $115.00. ISBN 1-56081-684-8.

This book consists of eight independent reviews that have as a central theme the chemistry of early d-block metal clusters supported by π-donor ligands. It represents a followup volume to *The Chemistry of Metal Cluster Complexes* (VCH; Shriver, Kaesz, and Adams, Eds.) which dealt mainly with later transition metals. Although there are many texts dealing with the synthesis, structure, and bonding of transition metal clusters associated with π-acceptor (e.g., carbonyl) ligands, there is a relative dearth of such works on the cluster chemistry of halide, alkoxide, amide, and related ligands. This volume, therefore, represents a timely addition to the literature.

The first chapter written by Cotton, Hughbanks, Runyan, and Wojtczak focuses on the octahedral halide clusters of zirconium although some related thorium systems are also covered. Both discrete molecular species as well as clusters contained in solid state phases are discussed. The major emphasis is on the underlying bonding principles that help rationalize the structural parameters.

The second chapter by McCarley deals with molybdenum oxide clusters. The material is neatly arranged according to nuclearity, finishing with infinite chains. The chapter is highlighted by many informative ORTEP drawings.

The third chapter by Saito covers the chalcogenide clusters of early transition metals. This chapter represents over one-third of the book and is an exhaustive review of what represents a significant area of

inorganic chemistry. All aspects of the synthesis, structure, and spectroscopy of these clusters is covered according to element. The chapter contains some extremely informative tables whose usefulness is increased by self-contained bibliography. This review will prove indispensable to anyone working in this area.

The fourth chapter reviews the book editors area of group 6 metal alkoxide clusters. The material is thoroughly covered with an important emphasis on reactivity. The chapter contains many useful figures of molecular structures and spectra.

The last two chapters by Haushalter, Meyer, Khan, and Zubieta focus on vanadium and molybdenum oxide clusters and units associated with phosphate and organophosphate ligands. Chapter five discusses the synthesis and structures of oxo clusters that are entombed within metal phosphate frameworks. Structural diversity is highlighted by both ball and stick pictures as well as polyhedral representations. In Chapter six the emphasis is on the use of organophophonates and organoarsinates as ligands for molybdenum and vanadium oxo units. The chapter emphasizes how small changes in the organophophonates or reaction conditions can lead to diverse structural motifs, some of which contrast markedly with those found in more traditional polyoxometalates.

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Transport Properties of Fluids: Their Correlation, Prediction and Estimation. Edited by Jürgen Millat (NORDUM Institut für Umwelt und Analytik GmbH, Kessin/Rostock, Germany), John H. Dymond (The University, Glasgow, U.K.), and C. A. Nieto de Castro (University of Lisbon, Portugal). Cambridge University Press: New York, 1996. xiv + 483 pp. $90.00. ISBN 0-521-46178-2.

The present volume was conceived by the Subcommittee on Transport Properties and the Commission on Thermodynamics of the International Union of Pure and Applied Chemistry as a complement to an earlier volume, *Measurement of Transport Properties of Fluids*, edited by W. A. Wakeham, J. V. Sengers, and A. Nagashima. The objective is to outline the principles that underlie the statistical mechanical theories of transport processes in fluids and fluid mixtures of nonelectrolytes in a way that leads to results that can be used for their prediction or representation and to give examples of how this has been implemented.

The emphasis in this work is on systems of practical significance, and the introductory part therefore includes some examples of the technological importance of a knowledge of the "traditional" transport properties, such as the viscosity, thermal conductivity, and diffusion coefficients, with which the volume is mainly concerned. The theoretical part is divided between chapters on dilute gases and gaseous mixtures, dense fluids, and the enhancements of transport properties that occur close to a thermodynamic critical point. For dilute gases, the basic methods of the semiclassical kinetic theory of monatomic and polyatomic gases are summarized and the structures of formulas for the transport coefficients in terms of effective collision cross-sections are then described. For dense fluids, the emphasis is on smooth hard sphere and rough hard sphere theories although there are also brief introductions to the corresponding states, absolute reaction rate, and free volume theories. Of the latter group, only the corresponding states method is developed at some length in later chapters. The chapter on critical enhancements naturally deals with behavior in the whole critical region rather than just asymptotically close to the critical point and draws on results from mode coupling theory. In the following part the correlation of data as a closed algebraic equation expressing a transport property in terms of the independent variables defining the thermodynamic state is discussed first in general terms and then with a practical example; advice on the use of equations of state in this context is also given.

The larger part of the remainder of the book applies all this introductory material first to selected methods and then to selected substances. Under methods we find accounts of the methods and results of computer simulation by equilibrium and nonequilibrium molecular dynamics, the use of the modified hard sphere scheme, the use of the corresponding states method, and a summary of various empirical estimation techniques. The selected substances include pure fluids of monatomic fluids, diatomic fluids, and polyatomic fluids (specifically, water and the refrigerant R134a). Nonreacting mixtures are represented by the archetypal carbon dioxide−ethane system and a separate chapter is devoted to dilute alkali-metal vapors as an example of a reacting mixture. The final part of the book provides an introduction to a number of data banks and prediction packages that are available for transport properties.

This is a comprehensive and up-to-date account of the best methods at present available for correlation, prediction, and estimation of fluid transport properties. The wide range of case studies from a large team of authors provides both a good picture of what can be done and also some accessible entries to how such things are done. It should find a wide range of users including both those working on the experimental determination and theoretical interpretation of transport properties and also those who need to use information on these properties in technological contexts.

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JA965733R

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Spreadsheets for Chemists. By G. Filby (Nuclear Research Center, FRG). VCH: New York. 1995. xx + 408 pp. $60.00. ISBN 3-527-28570-9.

If you are a busy chemist, swamped with work and data to analyze, help is in sight. Gordon Filby's book, *Spreadsheets for Chemists*, offers the working chemist, student, or chemical educator a simple, fast alternative to more complex or tedious methods of data analysis, while still maintaining the "feel" of traditional, hand-processing techniques. A high-density diskette that contains many Lotus 1-2-3 spreadsheets is also included with the book in order to give readers a fast start concerning the use of this versatile tool.

Unlike many computer books and manuals that, for many, are difficult to comprehend, Filby's book is easy to read and use. The only assumptions that Filby makes with respect to his target audience is that users have a general knowledge of what a spreadsheet program is and what they can be used for and some knowledge of the menus and submenus of the DOS-based Lotus 1-2-3 program. Although the use of a DOS-based spreadsheet program seems somewhat dated given today's Windows-based PCs, the ideas and techniques that are illuminated are readily applicable to any of the modern spreadsheet programs such as Microsoft Excel, Quattro Pro, or Lotus 1-2-3 for Windows. Further, Filby does devote some attention to such programs in Appendix B.

The book is divided into two main parts. Part I is titled The Mechanics of Spreadsheets. In this section, the reader learns the basics of spreadsheet data analysis such as performing simple arithmetic, graphing, adding titles, and the use of "built-in" functions, macros, branching commands, etc. After completing Part I, readers should be well versed in spreadsheet construction and data analysis using these methods.

More advanced readers who already know how to manipulate data with a spreadsheet may wish to turn directly to Part II of this book which deals with Applications in Chemistry. Fifty-seven different Lotus worksheets that illustrate applications from many different areas of chemistry are included in the book. All of these worksheets are also found on the diskette accompanying the book. To amplify understanding of ideas and analysis, readers are directed to attempt suggested "exercises" that are usually included at the end of each of these applications. If you are using a Windows-based spreadsheet, these worksheets are written in Lotus *.WK1 format and, in many cases, may be imported and converted directly into your Windows spreadsheet program.

In summary, *Spreadsheets for Chemists* is a "must" for all student or professional chemists who yearn for faster methods of data analysis but who wish to remain in intimate contact with the actual analysis process. The book is well written, easy to understand, and well illustrated by way of the accompanying diskette.

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JA955236V

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