spectroscopy in solution and by an X-ray crystal structure determination in the solid state.[7] **3** has an unexceptional 3-legged piano-stool structure with normal bond lengths and bond angles.

$$[CpFe(COD)][Li(TMEDA)] + PhCH_2X \xrightarrow[-TMEDA]{-LiX} [CpFe(COD)(CH_2Ph)] \quad (1)$$

1 **4**

$$[CpFe(COD)(CH_2Ph)] \xrightarrow[-COD]{DIPHOS} CpFe(DIPHOS)(CH_2Ph) \quad (2)$$

4 **3**

As shown in eq 2, the formation of **3** appears to indicate that the *initial* species formed in the reaction of **1** with $PhCH_2X$ was $CpFe(COD)(CH_2Ph)$, **4**. In the presence of DIPHOS, **3** was formed from **4** by ligand replacement. However, in the absence of a strongly coordinating ligand, **4** underwent disproportionation and reacted with TMEDA to form **2** and Cp_2Fe (eq 1).

Finally, the coupling product, $PhCH_2CH_2Ph$, was formed in minutes upon the addition of excess $PhCH_2X$ to a solution of **2** at 25 °C. This clearly established the intermediacy of **2** in the coupling of benzyl halides by **1**.

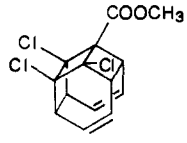
(9) Felkin, H.; Knowles, P. J.; Meunier, B. *J. Organomet. Chem.* **1978**, *146*, 151.

Registry No. **1**, 69393-63-1; **1**-Cp-d_5, 112440-11-6; **2**, 112440-07-0; **3**, 64827-29-8; $(TMEDA)_xFeCl_2$, 112440-08-1; $PhCH_2Cl$, 100-44-7; $PhCH_2Br$, 100-39-0; $PhCH_2Li$, 766-04-1; $PhCH_2CH_2Ph$, 103-29-7; benzyl-d_7 chloride, 59502-05-5; benzyl-α,α-d_2 bromide, 51271-29-5; benzyl-α-d_1 bromide, 66343-88-2; benzyl-2,3,4,5,6-d_5 chloride, 68661-11-0; benzyl-3-d_1 chloride, 112440-09-2.

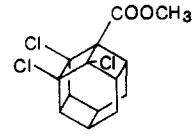
Additions and Corrections

Secohexaprismane [*J. Am. Chem. Soc.* **1987**, *109*, 2212–2213].
GOVERDHAN MEHTA* and S. PADMA

Page 2213: Structures **15** and **21** are missing one Cl atom each and the correct structures are as follows:



15



21

Page 2213, Scheme II, footnotes: Reagents and yields: (q) $HgO–CH_2Cl_2$ should read $HgO–CH_2Br_2$.

Computer Software Reviews

FORTRAN Package 2. Lektor, Inc.: P.O. Box 6713, Kennewick, WA. 77-page manual.

Lektor FORTRAN Package 2 is a collection of FORTRAN subroutines for a variety of numerical methods. The software is intended to run on an IBM PC or compatible with at least 256Kb of memory and two disk drives. A math co-processor is recommended. The software requires a FORTRAN compiler. Lektor suggests the IBM FORTRAN compiler, Version 2, or the IBM Professional FORTRAN compiler. These compilers require DOS, Version 2.00 or higher. The software is not copy protected; backing up the package is recommended by the vendor. The software consists of 34 source subroutines, as well as associated support routines and libraries.

The specific routines comprising the system perform the following functions: solutions to linear and nonlinear simultaneous and differential equations; numerical integration; interpolation; random number generation; special functions such as the error and γ functions and the exponential integral; the discrete Fourier transform; and an implementation of the Simplex algorithm. Since the software is distributed in source as well as object code, verification of the proper coding of the various algorithms can be accomplished by those wishing to do so.

The software is quite easy to use, as simple FORTRAN function calls are used, as

```
CALL SIMPS(N,FUN,A,B,ANS)
```

The limitation, of course, is for those who do not program in the FORTRAN language.

Various functions of the software were tested and found to operate properly. Although this package does not address particular chemical applications, it is a tool kit that can be readily applied to a number of problems of both industrial and academic interest. As with all numeric software, Lektor's caveat applies: "Because of the great variety of problems to which these service routines can be applied, no guarantee can be made... to the accuracy of any routine or its suitability for any particular application." For those in need of such FORTRAN software, this seems a complete and worthwhile package.

Brian J. McGrattan, *The Perkin-Elmer Corporation*

StatWorks. Cricket Software: 3508 Market St., Suite 206, Philadelphia, PA 19104. Retail price $125.00.

StatWorks is a software package designed for the Macintosh personal computer to provide an easy-to-use statistical analysis. Although the range of statistical procedures found in StatWorks is not as wide as that in a main frame environment, the procedures available are more than adequate for any statistical analysis or graphical representation which I have found necessary in my work as a chemist.

It is quite true, as is claimed in the Introduction to StatWorks, that statistical analysis on a personal computer often required wending one's way through a sea of often cryptic documentation or learning new higher level languages. This package contrasts dramatically from such procedures in that it can be easily addressed by anyone familiar with the simplest programs designed for the Macintosh (e.g., MacWrite or MacPaint). The philosophical goal of automatically taking the user through several stages to a complete statistical analysis without the requirement of creation of dummy variables is surely achieved.

The options for graphical representation of the data handled by StatWorks are the easiest methods I have seen for generation of tabular

representation of data. The program makes a wide variety of graphic outputs readily available. Since StatWorks performs all calculations with 19 significant digits, it does not suffer from inaccuracies due to round-off problems, at least so far as my test programs could address this question. The program also allows easy transfer of information from other Macintosh applications, i.e., from spreadsheets, terminal programs, etc. Graphs and statistical output may be easily transferred to reports created on the Macintosh via word processor.

Direct entry of data into the program is exceptionally easy. It is also routinely possible to cut or copy data from programs placed on the Macintosh clipboard from other programs, thus accessing spreadsheets or word processor-generated data. Transfer of data from a mainframe computer requires a terminal emulation program for the Macintosh. Transfer then occurs through the Clipboard from which data can be pasted directly into StatWorks.

Desk accessories and file menus are identical in StatWorks with the commonly available word processing programs designed for the Macintosh. The *Edit menu* differs from these programs only in providing an additional feature "grab picture", a command which copies the contents of a currently window to the Clipboard in picture format. This command can be used to transfer windows that contain statistical results or graphical plots. The *Data menu* in the program allows one to sort rows or an entire data set according to the order of a particular variable, and it can be done in ascending or descending order. It is possible to order with alphabetic as well as numeric data. The Recode option allows one to change one variable so that any cases with a value and a specific range are recoded into a single code, again either for alphabetic or numeric entries. The Transform command provides a handy route for mathematical transformation of raw data with the operations ln (x); e^x; x^n, where n can be non-integral and either positive or negative; sin (x); arcsin (x); or Z scores. A two-column transform command allows one to algebraically manipulate one variable by either a constant or another variable. This option can be used to weight data obtained from a sample survey, for example. Finally a command allows for a creation of random numbers that are used for various statistical purposes.

The *Stats menu* allows for parametric and nonparametric tests of data. Included on this menu are the most frequently used procedures for testing hypotheses about the mean of a single sample and comparing means of multiple samples. The descriptive statistics command tests the statistics of location and statistics of dispersion, describing respectively the central tendency of the sample distribution and the spread of the sample distribution. Automatically provided by this command are mean and standard error values, as well as calculated variance, standard deviation, and coefficient variation. The inclusion of Pearson's coefficient of kurtosis will undoubtedly be of more interest to statisticians than to practicing chemists. The cross-tabulation command computes the frequency of occurrence of all possible combinations of the levels between two categorical variables. A table is automatically created which displays a number of useful statistical values, including χ^2 and its significance level. The Student's t-test, the normality test, the Kolmogorov–Smirnov test, the Mann–Whitney U, the Wilcoxin signed rank test, the Spearman correlation test, and the Kendall correlation test are routinely available, but will probably be of more importance to statisticians than chemists.

The *Regression menu* provides three popular forms of regression analysis: simple, polynomial, and multiple. The simple regression involves the most basic regression model:

$$y = ax + b + \text{error}$$

In the simple regression mode, graphical depiction of the dependent and independent variables with the fitted regression line is accompanied by a statistical treatment of the coefficients and an ANOVA table. A residuals plot is also generated, which can serve as a useful diagnostic tool for checking the accuracy of the regression model. The polynomial regression involves a model expressed as

$$y = a_1x + a_2x^2 + a_3x^3 + \ldots + b + \text{error}$$

Similar data treatments are involved as in the simple regression. In the multiple regression mode, the model can be expressed as

$$y = a_1x_1 + a_2x_2 + a_3x_3 \ldots + b + \text{error}$$

Thus, many independent variables can be correlated with the dependent variable, through the same graphical depictions.

The ANOVA (analysis of variance) menu provide 1- and 2-weight analysis of variance techniques for samples with normal population distribution, and the Kruskal–Wallis and Friedman tests provide the analogous nonparametric counterparts.

Perhaps of greatest value to practicing chemists is the *Plot menu* which provides a wide variety of graphical displays enabling the user to plot 2 or 3 variables together as either scatter plots, line plots, histograms, 3-dimensional scatter plots, 3-dimensional histograms, or box and whisker plots. Axis intervals and labels are automatically determined and placed. One can select beginning and ending values and the interval whip for each classification. The plots produced by this menu are clean, easy to read and to control, and of publishable quality.

StatWorks thus provides a nearly complete range of statistical evaluation for data. The options available far exceed those normally needed by the practicing chemist, but even in these cases, the accessibility of the important data is easily attained. An inexperienced user familiar with the Macintosh can generate statistically analyzed plots within only a few minutes. The package is very powerful and one with which I am very impressed.

Marye Anne Fox, *University of Texas*

DataScan. Version 1.12. ISS Design: 531 West 8th Street, Plainfield, NJ 07060. List price $199.

It is often easier to perceive trends, deduce cause-and-effect relationships, and understand underlying phenomena when information is presented in graphical form instead of tabular data. On the other hand, numbers are preferred when results are being checked, when further calculations are required, and when results have to be stored for future reference. Graphical representation of information in a computer is more difficult than numerical data, but its value to chemists and other scientists is so high that we are seeing an increasing number of software products designed to both show and manipulate it.

The program DataScan for the Macintosh computer is an example of graphics manipulation. It takes a graphical representation and turns it back into a set of x,y numerical values. These numbers are placed in a disk file and can be used by other software for any purpose desired, such as database storage, curve fitting, peak detection, or use in modeling studies. DataScan is mostly useful when the original data that were used to produce a graph are not available. It is the reverse of a plotting program.

The program can be set to deal with line graphs, graphs of points, graphs that are filled between the x axis and the line, and bar graphs. When a plot consists of points and a best-fit line, the line can be removed if desired. The axes can be assigned for both linear and logarithmic scales. Both x and y grid lines can be automatically removed. They are not treated as part of the data.

The graphical information can be input to the DataScan program in one of several ways. An original or photocopy of the graph can be digitized by an appropriate scanner. DataScan supports Thunderscan, Microtek, AST, and Abaton digitizers. Sketches can also be drawn with the MacPaint program and used as input.

The graph has to meet certain requirements. The origin and y axis are used as reference points for DataScan and have to be well defined. The origin, for example, cannot have any tic marks, and the y axis must be straight and extend the full length of the graph. DataScan can compensate for a small amount of tilt, but it will fail if the original digitization was too far out of alignment. Grid lines parallel to the x axis can only be removed if tic marks exist at the y axis. If the inputted graph file does not meet these requirements, it must first be cleaned up with a graphics editing program like MacPaint.

DataScan has features that help it make the right interpretation and produce more accurate conversions to numbers. There is a smoothing function with selectable point count. The program can be set to ignore drop-outs in a line or isolated black marks up to a selected number of pixels. This helps reduce the effect of flaws in the digitization. These features can only go so far, however, and it is important that the inputted graph be of sufficient quality. Otherwise DataScan tries to include noise as part of the plot.

We found that a graph produced from a xerographic copy of a handbook page with a Thunderscan digitizer was so full of missing and false pixels that DataScan could not make any sense out of it. Even a simpler hand drawn graph was not interpreted correctly until we used the MacPaint program to clean up some extraneous marks and fill in small gaps in the lines. The time and effort needed to prepare the graph for DataScan to process is the most serious limitation. Because of this, we judge DataScan will only be useful when the need to convert a graph to numbers is sufficiently important and there are no better alternatives.

DataScan can be set to process graphs that consist of more than one data line. In this case, smoothing and some of the other features cannot be used if the multiple lines on the graph cross each other. On output, the numerical data are grouped by line segments that exist between crossover points. It is up to the user to determine which data set goes with which line after a crossover.

Sometimes the input graph file has much higher resolution than is needed and would produce too large of a list of output numbers. DataScan has an interpolation feature that allows the curve to be approximated with a fewer number of points. This routine does not space the

points evenly, but instead it clusters them to define sharp features of the plot and uses them sparsely when the line is flat. If too few points are requested, of course, important features of the graph will be lost. The user can experiment with different interpolations to get the best compromise.

The program works in two steps. The input graph is read in and receives some generic processing in pass 1. The user can then select different combinations of filters and interpretation functions to be applied before executing pass 2. After pass 2, a new display of the graph is presented so the effects of the functions can be evaluated. It is important to note that the enhanced plot produced here cannot be output to a file as an improved graph. There is a cursor with x and y numerical readout that can be moved around this graph. It can be used to evaluate features like peak tops or crossover points. Aside from that, the only purpose of the enhancing features is to improve the quality of the numerical data file produced by DataScan.

At first the manual was confusing. After we learned what the program was doing by running the examples supplied with it, the manual was much clearer. Computer documentation that does not make sense until after you know what it says is a common problem. In all, it took about 3 h to understand the program. DataScan runs reasonably fast and is easy to use. It makes clear and efficient use of the MacIntosh pull-down menu scheme. In one test, DataScan reproduced the original data used to make a graph with about 2% error. Presumably such accuracy depends on the care used and the resolution chosen during the digitization process.

Finally, it should be noted that the problem of turning graphs back into numbers is not trivial. Datascan does a reasonable job of dealing with the uncertainties and complications of this process. Those who have a digitizer and a need to make such conversions will find DataScan a very useful tool.

Robert Megargle and Robert Wilkes, *Cleveland State University*

Book Reviews

Polymeric Reagents and Catalysts—ACS Symposium Series 308. Edited by Warren T. Ford (Oklahoma State University). American Chemical Society: Washington, DC. 1968. viii + 295 pp. $54.95. ISBN 0-8412-0972-3

This book brings to the attention of organic chemists the usefulness of polymer-supported reagents. This volume contains only invited authoritative reviews. An overview by Warren T. Ford describes the history of polymeric reagents, including an account of Merrifield's solid-phase peptide synthesis and a brief short course on basic polymer bound Wittig reagents and a review on site isolation organic synthesis in polystyrene networks. David E. Bergbreiter describes useful chemistry which has been accomplished with use of soluble macromolecular reagents. F. J. Waller reviews the chemistry of NAFION resins and other perfluorinated ion-exchange polymers (PFIEP). Polymeric photosensitizers is the subject of a chapter by Doug Neckers of Bowling Green State University. John Ekerdt discusses the role of substrate transport in catalyst activity; Philip Garrou the stability of polymer supported transition metal catalyst; and Richard Taylor polymer bound oxidizing agents. Gunter Wulff reviews the literature on molecular recognition by imprinting with templates. Lastly, A. Patchornik co-authors a treatise discussing the future role of polymeric reagents toward automation in organic synthesis. The volume also contains an adequate subject index. In general, this ACS symposium series volume is well done and should become an initial reference text for any organic chemist contemplating using a polymeric reagent or catalyst.

James R. Zeller, *Parke Davis Company*

Rates of Phase Transformations. By R. H. Doremus (Rennselaer Polytechnic Institute). Academic Press: Orlando, FL. 1985. x + 176 pp. $29.00.

This book is intended as a graduate-level introductory text on the kinetics of phase transformations, with applications that could be of interest to materials scientists, chemical engineers, chemists, and physicists. The author has taken a broad point of view, emphasizing what is perceived to be phase-change behavior that is common to all materials. It thus seeks to present general principles rather than concentrate deeply on any particular type of application. There is a very brief introductory chapter on thermodynamics that does little more than define activities and activity coefficients. The second chapter is more thorough in its discussion of classical solutions to the diffusion equation with a Fickian diffusive flux in binary solutions, with particular emphasis on the solution to moving-boundary problems of importance in the study of crystallization and melting. There is also a brief description of interface and diffusion control and nucleation and growth, all in mathematical terms. The degree of detail and clarity of the presentation in this chapter is excellent. The author does a good job in explaining the physical implications of the formulas derived. There is a good set of homework problems at the end of the chapter, as well as bibliography separated into books and research articles. This practice is maintained throughout the remainder of the text, and it is a good way to get an introduction to the literature on specific applications of the material found in the chapter.

The third chapter deals with the thermodynamics of multicomponent systems, including surface energies. This is followed by a summary of the values of surface energies of solid surfaces, together with the implications of the surface energy terms as to the shape and size of crystals and the segregation of chemical components to an interface. Chapter four presents both theoretical and experimental results on the formation of liquid droplets from the vapor phase. There is a similar chapter (Chapter 5) on nucleation from condensed phases, both liquid and solid. This last includes a very clear explanation of spinodal decomposition, with a minimum of mathematics, but with very nice illustrations. Phase separation of liquids and crystal growth from the vapor are treated in Chapters 6 and 7. Chapter 7 is one of the more detailed treatments in the text, and it makes excellent use of the material in previous chapters on the thermodynamics of interfaces and the kinetics of nucleation. It also introduces the reader to the role of surface diffusion in crystal and whisker growth. Chapter 8 on solidification I found to be a little weak because the author does not go into a great deal of detail on the solution of the heat conduction equation with the required phase change boundary conditions, but rather chose to underline the importance of heat transfer in solidification using more qualitative arguments. The chapter does contain good descriptions of spherulite and dendritic growth and excellent plates illustrating the growth of solid crystals from the melt. The chapter on the growth of crystals from solution (Chapter 9) discusses the role of transport in the solvent on the crystal growth process and uses sucrose as the example for the formation of molecular (non-ionic) crystals. The growth of ionic crystals is briefly discussed, as is the effect of particle size on growth rates. However, this chapter does not consider in detail the strong influence of size distributions and impurities on nucleation phenomena. It would also have been nice to see some mention on the use of surfactants to control crystal growth (a common industrial practice) and some treatment of the crystallization of polyelectrolytes (proteins for instance). The last two chapters (10 and 11) are pretty much qualitative in nature, and they cover the growth of grain boundaries and precipitation in metals. As is true of the rest of the text, this material is also well-illustrated with pictures and diagrams.

This book is really a pedagogical masterpiece. It manages to get explanations of the main physical phenomena across with a minimum of mathematical detail, but with the use of excellent illustrations, photographs, and tables. The rigorous mathematical physicist may be disappointed, but this would be the book I would recommend to anyone wishing an introduction to the general area of phase transitions. The text is beautifully written. The exposition is clear, and when coupled with the carefully chosen examples and illustrations, it makes for fast, efficient and yes, even pleasurable, reading of some conceptually very tough subject matter. Finally, it contains a good index and, as was mentioned above, a good bibliography at the end of each chapter. This is an excellent book to be used as a text, or for the general scientist wishing a good introduction to the area of the kinetics of phase transitions.

R. G. Carbonell, *North Carolina State University*

Flow Injection Analysis: Principles and Applications. By M. Valcárcel and M. D. Luque de Castro (University of Cõrdoba). John Wiley & Sons: New York. 1987. x + 400 pp. $88.95. ISBN 0-85312-904-5

The popularity and utility of flow-injection analysis (FIA) is evidenced by the some 1600 publications on the technique in the past eleven years, nearly half appearing in the last two years. This monograph is a welcome English version of *Análisis por Inyección en Flujo*, published in 1984,

*Unsigned book reviews are by the Book Review Editor