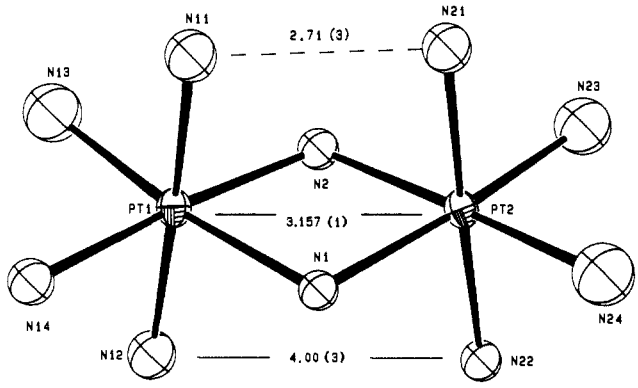

Figure 1. The structure and dimensions of $[(NH_3)_3Pt(NH_2)_2(H_5N_2)Pt(NH_3)_3]^{5+}$ as found in **1**. The N–H–N bond in the $H_5N_2^-$ bridge is represented by the dashed line: average Pt–N (terminal in plane) 2.08 (2) Å. Pt(1)–N(11), 2.03 (2) Å; Pt(2)–N(21), 2.06 (2) Å; Pt(1)–N(12), 2.08 (2) Å; Pt(2)–N(22) 2.14 (2) Å; average Pt–N (bridge) 2.08 (2) Å.

We have confirmed this assumption by a single-crystal X-ray study of $[(NH_3)_3Pt(NH_2)_2(N_2H_5)Pt(NH_3)_3](ClO_4)_5 \cdot 4H_2O$, compound **1**.[9] The structure of the complex is presented in Figure 1. Some striking features of this complex ion are revealed by comparing it with the fully protonated ion, as found in $[(NH_3)_4Pt(NH_2)_2Pt(NH_3)_4]Cl_6 \cdot 2DMSO$, compound **2**.[7] The separation between the two nitrogen atoms of the $(H_5N_2^-)$ unit is 2.71 (3) Å in **1**, compared with 3.30 Å between the corresponding nitrogen atoms in **2**. The Pt–Pt–N(H_5N_2) angles in **1** are approximately 84°, compared with 91° in **2**. This distortion is also reflected by the *increase* in the separation of the other two extra-planar nitrogen atoms from 3.30 Å in **2** to 4.00 (3) Å in **1** and of the corresponding N–Pt–Pt angles from 91° to approximately 98°. The considerable strain imposed by the H_5N_2 bridge also causes the collapse of the planar $Pt(NH_2)_2Pt$ configuration of **2**. The dihedral angle between the plane defined by Pt(1), N(1), N(2) and the plane defined by Pt(2), N(1), N(2) increases from 0° in **2** to 8.6° in **1**. The $(H_5N_2^-)$ bridging ligand has a very short hydrogen bond at its core; it is 0.5 Å shorter than the sum of the van der Waals radii of two nitrogen atoms[10] and therefore qualifies as a "very strong" hydrogen bond.[11] Further investigation of this hydrogen bond will be carried out by neutron diffraction, IR, and NMR studies. The role of the $(H_5N_2^-)$ bridging ligand in *ammine olation* (formation of μ-amido bridges) will also be studied. Evidence for the existence of *two* $(N_2H_5^-)$ bridges in the *doubly* deprotonated ion was obtained in a preliminary structural study of $[(NH_3)_3(NH_2)Pt(NH_2)_2Pt(NH_2)(NH_3)_3]^{4+}$.

Acknowledgment. We are indebted to the fund for Basic Research administered by the Israel Academy of Sciences and Humanities for financial support.

Supplementary Material Available: Tables of atomic positional and thermal parameters for **1** (3 pages). Ordering information is given on any current masthead page.

(9) Single crystals of $[(NH_3)_3Pt(NH_2)_2(N_2H_5)Pt(NH_3)_3](ClO_4)_5 \cdot 4H_2O$ were obtained by evaporation, at room temperature, of a solution of **2** which had been partly neutralized with NaOH to pH 5.6 (pK_2 of **2** is 7.1[7]). Compound **1** is triclinic, space group $P\bar{1}$ with $a = 9.564$ (2) Å, $b = 17.588$ (3) Å, $c = 9.464$ (1) Å, $\alpha = 91.95$ (3)°, $\beta = 119.32$ (3)°, $\gamma = 83.68$ (2)°, $V = 1379$ (1) Å^3, and $Z = 2$. The structure was refined by least-squares methods by using 3714 unique reflections with $I > 3\sigma(I)$ to a conventional R factor of 7.4%.

(10) Nyburg, S. C.; Faerman, C. H. *Acta Crystallogr., Sect. B: Struct. Sci.* **1985**, *B41*, 274–279.

(11) Emsley, J. *Chem. Soc. Rev.* **1980**, *9*, 91–124.

Computer Software Reviews

SuperPaint, Version 1.0 p. Silicon Beach Software: P.O. Box 261430, San Diego, CA 92116. List price $149.95.

SuperPaint is a graphics application for the Macintosh 512K, Plus, SE, XL and II. It occupies 161.5K according to the program information statement, yet when loaded with Switcher, it requires a minimum of 432K and prefers 614K memory. The application disk comes unprotected and can be used with 1 or 2 drives or with a hard disk. Although not designed specifically for chemical applications, SuperPaint would be very useful for creating publication quality drawings. It can input files not only in its own file format but also in the MacPaint format and the PICT format used by MacDraw and other applications. I have successfully transported graphics from MacPaint, MacDraw, and Excel.

SuperPaint has most of the features of MacPaint and MacDraw. Anyone who is familiar with these two applications will immediately feel comfortable with SuperPaint. I have found almost no feature in MacPaint and MacDraw that has been omitted from SuperPaint. The documentation describes SuperPaint as having two superimposed layers: (1) the draw layer, which is object oriented, and (2) the paint layer, which is bit mapped. The two layers may overlap or one may be hidden from the other. One can work in only one layer at a time, but can switch freely between them. Each layer has its own set of drawing tools, many of which accomplish similar functions.

The documentation is well written. It should be clear both to the experienced and the inexperienced Macintosch user. I found the index useful and adequately cross referenced.

Because SuperPaint combined many of the features of MacPaint and MacDraw, I will discuss mainly the differences. There are two sets of fill patterns available in both layers. One of these sets looks fine when printed on either the ImageWriter or the LaserWriter, the other looks fine on the LaserWriter. The latter set of patterns must be created in a draw layer, however, for best quality when printed. In both layers, one can draw circles, ovals, rectangles, and squares from their centers as well as from the rectangles that enclose them. Also lines can be drawn with different densities in the horizontal and vertical directions. One can rescale either objects or selected rectangles. Rescaling can either increase or decrease the dimensions of the selection. One has available three levels of magnification. In the paint layer, magnification works just like FatBits in MacPaint; however, in the draw layer, it allows positioning and reshaping of objects to the nearest pixel. Automatic scrolling is available when a tool is moved across a window boundary.

In the draw layer when an arc is created, it is drawn having a 90° opening. However, this arc can be edited to have any angle open. Polygons can be created with any number of vertices. Not only can one reposition these vertices but also one can increase the number of vertices as desired.

In the paint layer one can freely rotate a selected rectangle by any angle; the results are often distorted, however. One can also distort a rectangular selection in several ways not available in MacPaint.

SuperPaint allows one to create bit patterns for the LaserWriter at the 300 bit per inch (bpi) resolution. These objects can be edited just as if one were working in a paint layer, but because the screen resolution is only 72 bpi, the image will be an expanded view of what one would see on the LaserWriter. The LaserBits images can be transferred to either the paint or the draw layer. When displayed on the screen or printed on the ImageWriter, the images may be greatly distorted; however, when printed from the draw layer on the LaserWriter, the image prints with 300 bpi resolution. One can transfer images created at 72 bpi resolution (from the paint layer or MacPaint, for example) to the LaserBits editor, but they will be rescaled and, hence, considerably distorted.

Editing at the 300 bpi resolution is quite tedious, but the results can be quite dramatic. An example of the ACS emblem created in LaserBits is given below. I will give a copy of this emblem to anyone wishing to send me a blank disk (Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204). You will be able to paste this

printed from MacWrite

printed from Microsoft Word

into an application but you will need a copy of SuperPaint to edit it.

In summary, I found SuperPaint to be a very useful application for creating and editing graphics for use in chemistry.

William L. Switzer, *North Carolina State University*

Lotus MEASURE, Release 1. Lotus Development Corporation: 161 First Street, Cambridge, MA 02142. List price $495; educational discounted price $198 (minimum of 6 copies must be ordered). Requires Lotus 2.01, list price $495; educational discounted price $198 (minimum order of 6 copies). Upgrade cost from Lotus 1A to 2.01, $150, or $75 for 10 copies or more.

Lotus MEASURE is an add-on program for Lotus 2.01 spreadsheet (required), designed for data acquisition and instrument control. MEASURE is integrated into the Lotus program such that full access to all commands is easily achieved via the familiar Lotus command lines. The programs require an IBM PC, XT, AT, or compatible machine. This review was conducted on a Zenith 158 (8088-2 microprocessor), a Leading Edge model D (also 8088 based), and an ACER 1100 (80386, 16 MHz, based), with no apparent incompatibilities. A minimum of 640K of memory is recommended, with Lotus 2.0 being able to access up to 4 Mbytes of extended memory (EMS). MS-DOS 2.0 or above is required. While MEASURE is not copy protected, Lotus 2.01 uses an install/uninstall scheme, eliminating the need for a key-disk, but allowing the program to be installed on only one machine at a time.

MEASURE comes on two 360 K floppy disks with four independent modules, with support for (1) the IBM game port adapter, (2) IEE488 support (both NAT488 and HP488 drivers), (3) RS232 support, and (4) support for the Metrabyte DASH-16 data acquisition board. Installation is extremely easy. One simply follows the instructions in the manual, which are clear and complete. Installation consists of copying the driver files to a hard or floppy disk, creating a new driver set for the desired modules (achieved by copying the Lotus 123 driver to the new file), and then running a supplied program called NEWLIB, which completes the process. Installation required at most 5–10 min for all the drivers to be installed. Once installed, these modules are called by loading Lotus along with the desired drivers and then invoking their menus by an Alt-function key combination.

Lotus has developed an excellent reputation for their documentation, a reputation that is well-deserved. The Lotus 2.01 manual is well organized, with clear sections on accessing all of the spreadsheet functions. MEASURE meets these same standards, with a small "Getting Started" pamphlet which clearly outlines the installation and preliminary operation process, and a more comprehensive manual covering a Sample Experiment, with subsequent detailed chapters covering each driver. On-line help for Lotus is available through the F1 key, both for Lotus, and while a driver is invoked, for that particular driver. The Help facilities are excellent, so much so that a manual will hardly be needed.

The Lotus 2.01 spreadsheet offers many enhancements over the older 1A version, making it much more suitable for scientific work. The ability to utilize EMS memory, sparse matrix memory management, its automatic utilization of a math coprocessor, if present, the addition of regression functions, new logical functions, and other features such as easy to use graphics make Lotus an attractive general purpose laboratory tool. MEASURE helps to link these spreadsheet features to instrument control and data acquisition.

I was impressed with the power of this combination for control of RS232 and IEE488 type applications. For both of these interfaces, virtually complete control over the ports was possible, including baud rates, stop bits, parity, data word length, Xon/Xoff, break and timeout durations, incoming data parsing triggers, and concurrent captures from two or more ports (e.g., two or more RS232 or RS232 and 488 concurrently). Any instrument utilizing either of these types of ports can be controlled or accessed through MEASURE. The only limitations would be the degree of control that the instrument itself allows via these ports.

One of the least impressive features of MEASURE is the limited support of a single A/D board, namely the MetraByte DASH-16 board. I was not able to test data acquisition on this card, since I do not have one in the laboratory (I use instead a Data Translation 16 bit board). While the documentation seems to indicate the same high standards of full control and easy, menu-driven access to all of the important board functions, it was disappointing that Lotus chose to support only a single commercial board. In my opinion, this severely limits the versatility of Lotus as a general data acquisition tool. In our laboratory, which is heavily involved with chromatography, we would like to have been able to acquire analog data from various detectors and to perform statistical moment analysis on the peaks within a chromatogram using the logical and mathematical functions available within Lotus. The data could be exported in DIF files to other scientific programs, for further analysis and for graphical presentation on high quality plotters.

The retail prices of both Lotus and Measure are $495 each, for a total package price of $990. The educational discounted price would be $396, with the caveat that a minimum of 6 copies must be ordered. Except in a teaching environment, or a pooling on a University-wide basis of many researchers, this minimum copy order could be unrealistic. Thus, the individual researcher must expect to pay the full $990 retail, with discounted mail-order prices probably falling in the $700–800 range. This is still quite expensive when compared to other available software. If one requires general purpose A/D, D/A, and TTL type closures, programs, such as LabTech Notebook, Asyst, or Asystant+, should be investigated which offer more powerful and versatile features for less cost. These programs also allow for the exporting of data to Lotus via DIF files, so that one could gain the functionality of Measure in terms of spreadsheet manipulation of the data, albeit at a slightly higher total investment.

In the opinion of this reviewer, Measure, while an excellent program in many regards, is crippled by the support of only a single A/D board. For those who either own or intend to purchase this board, however, Measure is a "user-friendly", moderately powerful package. It should be noted that it lacks many of the very powerful features of the high-end data acquisition programs, such as Fourier Transforms. However, for the control of RS232, IEE488, and the IBM game control ports, MEASURE seems to be without equal in terms of ease of use, comprehensiveness, and overall power.

Richard A. Hartwick, *Rutgers University*

MINSQ, Version 2. MicroMath Scientific Software: 2034 East Fort Union Blvd., Salt Lake City, Utah, 84121-3144. Price: $179; multiple copy discount available.

MINSQ is a programming system for solution of nonlinear parametric equations. The system is designed to operate on an IBM PC/XT/AT or PS/2 and is available in four separate versions. The version ordered is based on the type of graphics card (Color Graphics Adaptor or Hercules Monochrome Graphics) and if math coprocessor support is desired. The system also requires a minimum of 512K ram and DOS 2.0 or higher for operation. For hardcopy, the MINSQ comes configured to support an Epson or IBM ProWriter printer and a Bausch and Lomb DMP-029 plotter. Information is given for configuring the system for other printers and plotters.

Scheduled additions to the system include modules for chemical kinetics, pharmacokinetics, differential equations, and Laplace transforms.

The 75-page manual fully covers each option available with the menu driven system. Algorithms used, types of information obtained, and strategies used in fitting data to a model are also discussed. Finally, the three tutorial data sets and models are presented. The files required for working these problems are found on the single disk provided with the system.

MINSQ is a menu driven program in which each option is selected via function keys. As options become available during the execution of the program, they are added to the menu. Initially, the user must either retrieve a model from disk or enter one using the keyboard. Existing models can be edited as well. To create a model, the user must first list all independent/dependent variables and parameters to be used. A series of equations to be fit is then entered. Equations are then entered using standard equation formats found in BASIC, FORTRAN, or Pascal. Functions common to these languages such as ln, cos, and sin are supported. Integral and derivative functions are also supported. Once a model has been created, data can be entered from disk or manually along with initial estimates and ranges for parameters. Once all of this information is available, it is then possible to conduct a fit of the data.

Data can be fit using either a Simplex or least-squares (Levenberg-Marquardt) algorithm. Options for simulating a fit, adjusting the weighting of data, and using only a subset of the data/parameters fine tuning of the fitting parameters (step size and sum of squares goal) can also be controlled. After using the least-squares option, statistics related to the fit of the data can be displayed including confidence ranges, variance, and analysis of residuals.

An extensive graphics subsystem is provided with MINSQ which allows for data and calculated curves to be displayed as X–Y plots. Plots may be stored, retrieved, and edited to produce publication quality plots. The graphics editor allows for resizing plots, rapid addition of lines, arrows, and text (using one of several fonts provided), and moving/removing any added objects. Options for printer and plotter output are also provided.

Unlike other scientific data analysis packages, MINSQ is designed to do only one thing, fit nonlinear parametric equations. As a result, it is simple to learn and use and the manual is clear and concise. The menu driven user interface is consistent, only presenting options as they become appropriate.

James K. Hardy, *University of Akron*

MINSQ and RSTRIP, Versions 2.1 and 3.0. MicroMath Scientific Software: 2034 East Fort Union Blvd., Salt Lake City, Utah 84121-3144. List price: $179 each; $329 for both packages.

MINSQ is a fitting package designed for use with an IBM or compatible computer. RSTRIP is a complimentary package of fitting routines designed for pharmacokinetic applications (other packages are due to be available for use with MINSQ). The programs are not copy-protected; however, the software is sold for use on a single computer (site-wide licenses are available). The packages are warrantied for 90 days and no indication is given as to customer support or prices for updates.

Documentation: The manuals provided with both packages are very basic and provide the necessary information to use the package. In addition, a file is provided that includes the current updates. The introductory chapters provide a good summary of the software capabilities and the examples are well chosen for the chemical user. The major fault lies in the lack of detail in the fitting routine methodologies. The user must have some statistical background or consult the references listed to fully appreciate how the fits are performed.

Installation: The current version was installed on a hard disk drive and configured with the reviewer's desired hardware (not the default). This was readily accomplished (~10 min) and should be possible for most common systems. The configuration file is easily modified, and several format files for printers/plotters are included.

The evaluation of the software was made using an IBM, PCAT, CGA monitor, 8087 co-processor, HP7470A plotter. The software takes up two floppy diskettes (about 650K hard disk space) and is compatible with monochrome, CGA, and EGA adapters (the minimum requirements are 512K RAM and 2 floppy drives or a hard disk).

Usage: Both packages are menu driven and include utilities that are available separately (Directory Window, $15.95). This allows one to perform several DOS commands from menus.

The program on the whole is rather simple to use, with all features easily accessed via the menus. This makes it attractive for a novice in the area. It suffers from some major limitations that will restrict its usage in the current version: (1) maximum number of data pairs = 100; (2) limited number of plot options (the reviewer tested the system on an HP7470A plotter), e.g., symbol selection; additionally, no option for residual plots is provided; (3) errors/subtle mistakes return the user to DOS (there are no indications in the documentation as to what the error codes mean).

As a whole the ease of use (at all levels, particularly model/data input), the large number of operations allowed (including itegration and differentiation), and the detailed statistical output make it an attractive package as a teaching tool and/or starting package. However, the drawback and cost (compared to more extensive packages available) limit this versions usefulness to the general scientist.

The reviewer compared the perfórmance of this software package (with data collected in these laboratories and generated exponential decays) with his own (written in BASIC, using a Marquardt based algorithm). For a simulated double exponential decay with 100 points, the MINSQ software found two "false" minima before finding the correct solution (~30 iterations, 2 min). The reviewers' algorithm found the minimum (starting with the same initial guesses) in ~20 iterations, in ~30 s.

The accompanying RSTRIP software (along with other planned application sets) is a "neatly" packaged module and easy to use. Its moderate cost makes it attractive to the industrial community. However, similar results can be obtained from the MINSQ package (with some effort) and limits its use to the chemical community.

Michael Albin, *California Institute of Technology*

Book Reviews

The Handbook of Environmental Chemistry. Volume 4. Part A, Air Pollution. Edited by O. Hutzinger (University of Bayreuth). Springer Verlag: Berlin, Heidelberg and New York. 1986. 222 pp. $76.50. ISBN 0-387-09688-4

Five authors have each contributed one chapter to this first part (A) of the series on Air Pollution (Volume 4). The editor and four of the authors represent three different European countries so the book has somewhat continental flavor, although air pollution science is clearly, at least in the developed world, quite universal. Except for the first chapter, each topic is directed toward a professional audience with an interest in the particular subject. Thus the book is neither a handbook compilation of reference data nor a text on the subject of air pollution.

The first and shortest chapter (22 pages) by A. Wint of the University of Nottingham, England, is an overview called "Air Pollution in Perspective". It is quite nontechnical with only one chemical equation, three tables, and no mathematics. The table of contents for this chapter reveals that air pollution is discussed in global, regional, and local terms. The point is made that an earlier age tacitly assumed that the atmosphere was so huge that it could absorb and dispose of all our gaseous waste. In recent decades the view that only those living very near air pollution sources would be affected has been totally discarded. Later sections of this chapter deal with adverse impacts on health but in a very cursory way in such a short chapter. Vegetation damage is virtually ignored.

The second chapter, by P. Fabian of Max-Planck-Institute für Aeronomie, FRG, is titled "Halogenated Hydrocarbons in the Atmosphere". This chapter, in 29 pages, summarizes current data on twenty of these compounds, many of which are important both technologically and as air pollutants. Data on atmospheric levels as well as trends in emission strengths are given through about 1982. Almost all references are this old or older. With the intense current interest in the role that this family of compounds plays in the ozonosphere, especially in the now famous antarctic ozone hole, it would be difficult to keep up to date on this topic. The chapter does not attempt any review of the vast literature on modelling of the ozonosphere and its depletion.

Hans Güsten of the Institute für Radiochemie, Karlsruhe, FRG, contributed chapter 3 on "Formation, Transport, and Control of Photochemical Smog" (52 pages). This topic is perhaps more mature than the halohydrocarbons since it dates from the pioneering work of A. J. Haagen-Smit in 1950. "Smog" symptoms have now been found in many cities around the developed world and since lifestyles have become so similar the resultant urban smog varies mostly in severity due to population and meterology. This chapter is a good survey of current understanding of smog although each of the three topics promised in the title could by itself take up a good sized book. This means that some very important topics such as automotive emission control receive very short coverage. In fact "formation" including discussion of products gets the largest share of this chapter.

"Atmospheric Distribution of Pollutants and Modelling of Air Pollution Dispersion" by H. van Dop of the Royal Netherlands Meterological Institute, the Netherlands, makes up Chapter 4 (42 pages). The article is written from a meterological perspective and begins with the basics of atmospheric physics and dynamics and proceeds through the modelling of dispersion to culminate in a source/receptor matrix for Europe (Table 6). This gives the calculated sulfur deposition in each European country from every other country.

The last chapter, by J. M. Hales of Battelle Pacific Northwest Laboratories, USA, is titled "The Mathematical Characterization of Precipitation Scavenging and Precipitation Chemistry" (74 pages). Removal of pollutants from the atmosphere by precipitation is good news/bad news. If there were no removal mechanism pollutants would accumulate indefinitely. Yet this process leads to acid rain (precipitation) and fallout with impacts that are far from being understood. As promised in the title, this chapter is quite mathematical although the author says his presentation is highly "visual" so the reader can recognize the relationships between the physical process and their mathematical description. To see how successful the author has been the reader would need to study the mathematics in detail. In one footnote the reader is encouraged to use Laplace transforms to solve a pair of simultaneous partial differential equations. The final section gives advice on model selection, a list of references to special models, and some comparisons with observations.