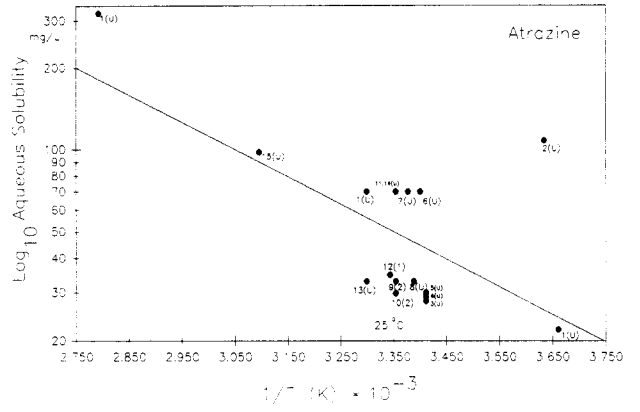

Figure 1.

(such as the HP LaserJet). Optional pointing devices include a mouse and an electromagnetic tablet.

Installation of the program was simple and was completed without a problem. I installed the system on drive D. The installation program has the nice feature in that the system can be reconfigured (for example, to change the type of hardcopy output device being used) without having to reinstall the entire system. The program worked the first time I started it up. The manual is generally very good, with all the needed explanation either in the body of the text or in an appendix. There are 10 tutorials, very clearly described in over 90 pages of text. These are excellent.

By the end of the first morning I installed the program I was able to turn out graphs such as in Figure 1, which is a plot of the log of the solubility of the pesticide atrazine as a function of 1/temperature in kelvin. This plot, using an HP LaserJet Series II printer, shows a number of the features of Sigma-Plot, but also points out some minor problems. There are 15 points on the graph, but the labeling capability is currently limited to 20 items. (I was told this will change in the next release.) This required some manipulation of the labels, such as having to put more than two labels in one item line. It would be nice to have a larger number of lines available for labels. It is possible to patch together two graphs on top of one another, using the compose option, and get more than 20 labels, but it is a bit of a kluge. Another bothersome item with the program is that when the data are entered into the program, Sigma-Plot automatically uses three significant figures, no matter how many are entered. Thus, a temperature of 25 is 25.000, and a value of 0.1234 is 0.123. I was told this also would change in the next release. Using simple commands, one is able to rotate a label, enlarge it, or reduce it. Right, left, and center justifications are available. For those with color plotters, one can make amazing technicolor plots.

The program is divided into modules; one first does data entry and then goes on to plotting, graph editing, replotting, reediting, and finally saving a result. The modules or menu choices include the main menu, disk menu, edit menu, compose menu, options menu, edit graph menu, exit axis (x or y) menu, and the edit plot menu. Moving back and forth is quite rapid and particularly easy with a mouse, but the function keys are almost as fast and convenient. Moving labels on a graph is easily done with the arrow keys. The only problem is the difficulty in seeing where a point or label is on the screen to ensure the plot is exactly where it is wanted. Since the laser printer and plotters are of such high resolution relative to a PC graphics screen, I am not sure this problem can be solved. As the plot on the HP laser printer takes about 1 min (more or less, depending on the number of points, the complexity of the graph, and the memory in the LaserJet printer used) to print, I find this need to make a few final plots a very minor issue. In any event, I have discovered through using Sigma-Plot that everyone has a personal view on exactly where a label should go since it is so easy to redo a graph. One other plotting feature that is very nice, but available only with a laser printer, is the ability to vary the width or thickness of a line.

Sigma-Plot allows for curve fitting, with up to 10th order polynomial regression. The graph in Figure 1 is a simple log plot. Error bars can be added to a point on the graph. Two graphs can be put on a plot, or, put another way, one can have multiple plots on one graph. Math and Greek symbols are available. There are a wide variety of thick-mark capabilities (e.g., major and minor) that are possible. One can even prepare slides comprising just text.

Whenever I had any questions, there was an 800 toll-free number to call, and problems were quickly solved. I called on four occasions, at different times of the day, and always found someone to answer my question, even if the problem would not be solved with the current version of the program. I would rate the support as excellent. Jandel also has a free bulletin board for Sigma-Plot and their other products, but the user must pay for the phone call. The program error messages are clear and easy to understand. The program is full of error checking and tries to keep the user from doing stupid things, like deleting data that was not saved. Overall I was very pleased with the software and have been using it regularly. I would recommend it to anyone with an IBM PC or clone who needs easily generated publication-quality graphs.

REFERENCES AND NOTES

(1) Available from Jandel Scientific, 65 Koch Road, Corte Madera, CA 94925 [(415) 924-8640 or (800) 874-1888; FAX (415) 924-2850]. Price is $495.00. It is expected that version 4.0 will have the same list price as version 3.1 reviewed here.

Janssen Chimica Catalog with HTSS

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Janssen Chimica, a distributor of laboratory chemicals, has put their chemical catalog of over 10 000 chemicals on a set of floppy disks for distribution using the Foxbase database management system software.[1] What makes this package interesting is that they have combined, for an additional cost, a chemical structure search capability, using a modified version

0095-2338/89/1629-0290$01.50/0

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Janssen Chimica catalogue of fine chemicals
for research and industry

Product number 13.182.87

Name           2-PYRIDINECARBOXALDEHYDE 99%

Mol.form.      C6 H5 N O
CAS-nr         1121-60-4

Packages       25      GR    11.00 USD
               6X 25   GR    10.00 USD
               100     GR    28.80 USD
               6X 100  GR    26.00 USD

(N)ext, (P)rev, p(H)ysical or s(A)fety data, (O)rder, (R)esume or (S)top
```

Figure 1.

of the HTSS PC structure search software package from ORAC Ltd.[2]

The entire package comes on 11 360K floppy disks, with manual of about 130 pages (split between the chemical catalog and HTSS), requires about 12 MB of hard disk storage, MS or PC-DOS version 2.1 or higher, and (for using the HTSS software) an EGA or a Hercules graphics board and a Microsoft or equivalent mouse. Only the HTSS portion of the manual has an index. The installation of both the catalog and the structure search system took about 30 min. While the installation instructions were clear, they were not completely accurate. Thus, when I finished the installation, some of the program functions did not work at first. This was due to my choosing an option in the installation procedure to split the files on two disks, C and F. I did this because my C disk was rather full, and the instructions said it could be split. After two FAX's back and forth to Belgium, I was provided with the necessary information to have the system work the way I needed it to work on my system. It involved a simple batch file and the reassignment of drives. While the response to my problem was quick and helpful, it would be better to build in the complete and accurate installation procedures into the manual and programs. A further problem arose later when I tried to print the screen to have a diagram for this review. The print procedure was not included in the modified version of HTSS included with the package.

The search capabilities of the data in the catalog are good. One can search by Janssen product number, chemical name, partial chemical name, molecular formula, and CAS Registry Number. After a search is completed, one can display the chemical information from the catalog, including the amounts in which it is sold and its price (as of the catalog publication), as well as physical and safety data on the chemical. The physical data include (subject to availability) melting point range, boiling point range, index of refraction, density, and optical rotation. The safety data include fields like waste disposal, flash point, RTECS number, and Sax reference. None of the contents of the 46 files, described on pages 16 and 17 of the manual, are defined. While some are obvious (e.g., name, molform, or density), others were not so obvious to me (e.g., brether, riskadv, propc, eeglab1, or eeglab2). In a similar fashion, the display uses the term "retecs", which is incorrect. The abbreviation for the U.S. government database called the Registry of Toxic Effects of Chemical Substances is RTECS and should be all upper case letters.

One can browse through and search the catalog and even prepare an order for chemicals using the system. The latter

```
                    Safety Information - Screen 1

Product Number      Retecs Number       :
  13.182.87         Flash Point         : +054
                    Autoignition Temp   :

----- Waste Disposal -----
   Disposal should be in accordance with local, state or national
legislation. The compound should be burned in an incinerator equipped with
an afterburner and a scrubber. Ideally, all hydrocarbons and related
solvents should be burned in a solvent incinerator. Halogenated compounds
should be ignited in the presence of sodium carbonate and calcium hydroxide
(slaked lime). The solid or the liquid absorbed on vermiculite should be
mixed with the dry caustics, wrapped in paper and burned in a incinerator.

                    (N)ext screen, (R)esume
```

Figure 2.

```
                    Safety Information - Screen 2

 Product Number     Hazard Symbols     Sax Ref.  Bretherick Ref.
   13.182.87              C

----- Risk Description : R(10 34) -----
  Flammable
  causes burns.

----- Safety Advices : S(3/7/9 28 36) -----
  Keep container tightly closed in a cool, well-ventilated place.
  After contact with skin, wash immediately with plenty of .....
  Wear suitable protective clothing.

                    (P)revious screen, (R)esume
```

Figure 3.

```
                    Physical Information

      Product Number          : 13.182.87
      Melting Point           :
      Boiling Point           : 181.00 - 181.00 (760 MM HG)
      Index of Refraction     : 1.54
      Density                 : 1.1260
      Optical Rotation        :

                        (R)esume
```

Figure 4.

is really just a list of what you want with your name and address along with the name and address of whom to send the invoice to. Browsing through the catalog using the CAS RN, molecular formula, or name is easy and will often find entries that would not be found otherwise.

Once a chemical of interest is found, the program displays the main entry information, shown in Figure 1, which consists of the chemical name, molecular formula, CAS RN, and the sizes and costs of the packages available from Janssen. From there one can display the physical properties and safety data available on the chemical. This information is similar to the Material Safety Data Sheets (MSDS) available from a number of U.S. chemical supply houses, but not as detailed as that available from MSDS databases such as distributed by J. T. Baker and Aldrich. I would hope Janssen would expand these data in future releases.

REFERENCES AND NOTES

(1) Available from Janssen Chimica, Turnhoutseweg 30, B-2340 Beerse, Belgium (telephone, 32-14-60-21-11; FAX, 32-14-60-28-41). Price is $1000.00 for the catalog and $2150.00 including HTSS.
(2) Maxwell Communications Corp.-ORAC Limited, 175 Woodhouse Lane, Leeds LS2 3AR, U.K. (telephone, 44-532-441821; FAX, 532-448283).