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****** CALCULATE VAPOR PRESSURE. ******

    62-53-3 C6H7N       aniline
                        aminobenzene
                        benzenamine
                        phenylamine
REFERENCE : 1973
 Boublik,T. ETC. 'THE VAPOR PRESSURE OF PURE SUBSTANCES',NEW YORK,1973
INPUT TEMPERATURE(K) : initial=300 final=500 increment=20

TEMPERATURE PRESSURE  STATE COD RAT   TEMPERATURE PRESSURE  STATE COD RAT
   (K)       (kPa)                      (K)       (kPa)
---------------------------------- ----------------------------------
  300.000            Out of range       320.000            Out of range
  340.000            Out of range       360.000            Out of range
  380.000   8.151      L   I   B       400.000   17.53      L   I   B
  420.000   34.55      L   I   B       440.000   63.33      L   I   B
  460.000            Out of range
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Figure 1.

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****** SEARCHING FOR COMPOUNDS WITH GIVEN TEMP. & PRESSURE. ******

INPUT:Temp.(K)=250 Pres.(kPa)=100 Tol.(kPa)=10

1       74-87-3 CH3Cl       chloromethane
                            methyl chloride
                            methane, chloro-
  State: L   Temp.(K)= 250   Pres.(kPa)= 106.006

2       74-99-7 C3H4        propyne
                            1-propyne
                            methylacetylene
  State: L   Temp.(K)= 250   Pres.(kPa)= 100.793

3      115-10-6 C2H6O       methoxymethane
                            dimethyl ether
                            ether, dimethyl-
  State: L   Temp.(K)= 250   Pres.(kPa)= 109.125

.
.
.

13    7291-09-0 C2H6Si      vinylsilane
  State: L   Temp.(K)= 250   Pres.(kPa)= 98.9719

    13 compounds found from 5766 records in the file.
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Figure 2.

desired.

The system came on one 3-1/2-in. floppy disk and took a matter of seconds to install on my hard disk. (It is also available on 5-1/4-in. 360K or 1.2 MB floppy disks.) The system requires an IBM or equivalent with PC or MS DOS version 2.0 or higher and about 1.2 MB of hard disk space. A printer is needed if you want to print out the results of a search or retrieval. The program started right up and worked without any problems. The system capabilities include searching chemical name(s), searching by molecular formula, and searching by CAS Registry Number. There are HELP messages throughout the program, which is a very nice feature. All search results described below are stored in a file and can be printed out at the end of a session.

There are three main system options, Retrieve, Search, and File. The Retrieve option allows one to retrieve a chemical by name, molecular formula, or CAS Registry Number and then calculate the vapor pressure for that specific chemical over a specified temperature. For example, Figure 1 shows the results of a search for aniline. This search was made by use of the name option (the same answer was found when the molecular formula option was used), and then the vapor pressure over the range 300–500 K in 20 K increments was asked for.

In the Search option one is asked for a temperature, pressure, and increment. The example in Figure 2 is for all compounds with a vapor pressure of 100 ± 10 kPa at a temperature of 250 K. There are 13 compounds whose vapor pressures at 250 K meet this criterion, and the first three and last one are shown in Figure 2. The system allows for a variety of units of both temperature and pressure. The temperature units allowed are Celsius, Fahrenheit, and Rankine. The allowable pressure units include pascal, bar, Torr (mmHg), inches of Hg, atmospheres, kg/cm^2, and lb/in.^{2}.

The File option allows one to Review, Print, and/or Save the results of previous searches. Even though I have a 386 CPU machine with 4 MB of main memory (640K of DOS accessible memory), I always got an error message that there was "not enough memory to open window", so I was unable to review the results of previous searches. The Print option worked just fine, as did the Save option. I used the Save option to save the results of searches and edit them for the material included in Figures 1 and 2.

There are a few bothersome points that I hope the authors will fix in their next release. For example, for a CAS Registry Number search for 1912-24-9, which is atrazine, the most widely used pesticide in the U.S. today, the system responds "No such compound". One gets the same answer for a search for atrazine using the name search option. I would think "This compound is not currently in the database or no such compound exists" would be a better message. As the program is case dependent (why it is in this day and age I cannot imagine), a search for aniline using c6h7n results in the message "formula pack error", requiring one to re-enter the data as C6H7N to get a hit (actually four hits as there are three other chemicals in the database with this same formula).

The system comes with a nice, short, 11-page manual, which is clearly written and easy to understand. For people who need vapor pressure data, this is an excellent, easy to use way to get it, assuming the chemical needed is one of the 5766 in the database.

REFERENCES AND NOTES

(1) Available from TRC Data Distribution, TEES Business Office, Mail Stop 3124, The Texas A&M University System, College Station, TX 77843-9988 [(409) 845-4940; FAX (409) 845-9267]. The price is $550.00.

Sigma-Plot, Version 3.1

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Sigma-Plot[1] is an IBM PC (XT, AT, or PS/2 and equivalent) based package for creating publication-quality graphics in conjunction with a high-resolution printer or plotter. The version reviewed here is 3.1, but version 4.0 is expected to be available by the time this review is printed. Sigma-Plot comes on seven 360K floppy disks with a manual of about 250 pages and requires about 0.5 MB of hard disk storage for the basic programs, 512 (or 640K depending on your system configuration) kB of memory, MS or PC DOS 2.1 or higher, CGA, EGA, VGA, or Hercules graphics card, and a plotter or printer

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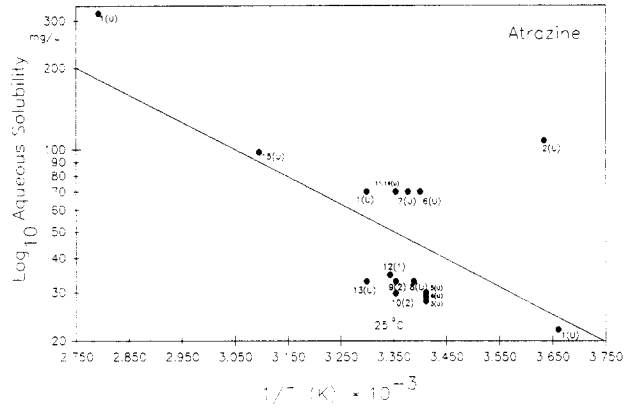

Figure 1.

(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

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