The 1984 Pittsburgh Conference: A Special Instrumentation Report

The 35th annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy continued its remarkable growth. This year's attendance totaled 24,648, a 13.5 percent jump from 1983. Nearly 800 of those were students. Some 636 companies occupied 1607 booths, both increases of about 9 percent. Part of the growth could be attributed to an increased foreign presence among both exhibitors and conferees. Several companies from Australia, for instance, were present for the first time. Beyond the hoopla over laboratory software, there were few discernible trends at the show. There were a few more molecular biology–oriented instruments, a few more instruments with the capacity to diagnose their own defects, and, because of increased use of computer workstations in the laboratory, a small number of instruments with no knobs, keyboards, or screens began to appear. This last trend may die aborning, however. Says one salesman who insisted on anonymity: "Chemists like to have something on the instrument to fiddle with."

Personal Computers Attract Lab Software

As the computerized laboratory evolves, most forecasters are touting the idea of a distributed computing network. A laboratory workstation built around a powerful 16- or 32-bit microcomputer is an essential ingredient in this scheme. The workstation can control several instruments, can gather data from the instruments and analyze them, and can pass appropriate information to larger computers in the network that are responsible for overall laboratory management or can receive instructions from these computers. "The time has arrived when the scientist has at his desk a computer with all the power he needs," Frederick Putnam of Laboratory Technologies Corporation told *Science*.

In parallel with this evolution, scientists have been bitten by the personal computer bug along with everyone else. As a result, laboratories are crawling with the various versions of the Apple II and increasingly with the IBM PC, by far the two most popular models of the personal computer. The upshot is that, in pondering how to automate their laboratories, scientists possessing Apple and IBM personal computers have discovered they have the makings of a workstation already in hand.

This situation has opened the way for a new wave of laboratory automation software written for these two personal computers to complement the enormous amount that exists for other purposes. Along with this trend, numerous instrument manufacturers are now offering controllers and data stations built around these personal computers rather than specially built dedicated machines or larger minicomputers.

A number of these companies exhibited their wares at the Pittsburgh Conference. Nelson Analytical is a scientific software house that was started up about 4 years ago by ex–Hewlett-Packard marketing manager David Nelson. Not surprisingly, the company specialized in software to run on Hewlett-Packard machines. The software itself is for the automation and management of chromatography laboratories. Last August, Nelson Analytical introduced its Model 3000 multi-instrument data system for gas and liquid chromatography for the IBM PC. "Two winners. Our chromatography software and the IBM Personal Computer," trumpeted an ad in a magazine distributed at the conference.

The reasoning behind the switch, according to John Blunden, a sales manager at Nelson Analytical, starts from the observations that the IBM PC is a reasonably powerful machine and that it is already in many laboratories. Since it may have been bought originally for other purposes, its use to automate a chromatography laboratory is a big bonus. "We expect a lot of business selling software and interfaces," says Blunden.

The Model 3000 can simultaneously handle up to six chromatographs with two detectors each, even with each instrument connected to an autosampler, while running off-line programs unrelated to chromatography. The software, which includes the same features as previous Nelson Analytical chromatography offerings, is written in BASIC. An interface device that collects data from the instrument and passes them on to the computer, either immediately or after temporarily storing them, is also included. Blunden says costs are typically of the order of $6,000 if the buyer already has a PC and $11,400 if not.

Dynamic Solutions Corporation (DYSC) has been personal computer–oriented from the start. Its products are designed to run on Apple II+ or IIe machines. According to David Strand, the president of DYSC, the company's software is aimed at the scientist who already has laboratory instruments but does not have extensive data-handling capability. The idea is also to make the software, which has the generic title Appligration II, as easy to use as possible. The user makes his way through by means of the now nearly universal menus displayed on the video monitor. "We are trying to extend the business spreadsheet capability into the scientific world," says Strand.

DYSC software comes in three forms. The Appligration II Starter Set contains certain hardware enhancements to be added to the user's existing Apple computer so that the software will run. The user can construct programs from a library of quite powerful commands. Only one command, for example, is needed to detect peaks and correct the baseline of a spectrum. Rather than programming every detail of a procedure, the user need only string together a sequence of these commands in the desired order. Cost of the starter set is $1995.

In addition, there are four application software packages for chromatography, continuous flow colorimetry, spectroscopy, and thermal analysis, which cost $495 each. A unique feature of these programs is the ability to scroll through graphically displayed data. The user can

pick parameters off the display to enter into the analysis. For example, baselines can be selected by means of a cursor. Finally, there is an expansion package for the starter set library at $395. In all three cases, listing of the BASIC programs are provided so that the scientist understands and can modify data-handling procedures if desired. It is also necessary to have a data acquisition or interface system. DYSC recommends several or will sell its own for $975.

Cyborg Corporation, has been turning personal computers into laboratory and industrial workstations for several years. Its line of ISAAC data acquisition and control systems to mate Apple II+ and IIe computers and various types of instruments has been available about 5 years. More recently, the company introduced the ISAAC 2000 system, designed for the IBM PC.

According to J. Michael James, a vice president at Cyborg, the personal computer phenomenon benefits both customers and software companies. A data acquisition and control system from any of the big instrument companies or from Cyborg will have comparable capabilities, but Cyborg gives you a personal computer and all the other things you can do with it. At the same time, no one company can write software to cover every conceivable use for a personal computer, so imaginative software writers can create products with potentially large markets, such as laboratory automation.

The ISAAC 2000 is built around a microprocessor (Motorola 68000) that is just as powerful as that (Intel 8088) in the IBM PC. In short, the interface between the PC and the instrument is far more than just a few simple circuits and a cable. Among its capabilities, the ISAAC 2000 can receive data at rates up to 200,000 samples per second divided among one to four input channels. And it can store up to 2 megabytes in its buffer memory. Up to 14 ISAAC modules can be connected to one PC. Finally, ISAAC can be controlling the instrument and acquiring data independently, while the PC is busy on other tasks.

The system is programmed by the user in a modified form of BASIC that has had a large number of data acquisition commands added to it. The older Apple-based systems also offer software packages for chromatography and for data logging from thermocouples. According to James, typical costs are about $6000 for an Apple-based and $9000 for an IBM-based system including the computer, and about half those amounts without the computer.

Keithley DAS exhibited a very similar data acquisition and control system for Apple II+ and IIe and IBM PC computers, the Series 500. The company is a joint venture, formed last October, between Keithley Instruments and Data Acquisition Systems. An extra wrinkle added by Keithley DAS is the marketing of applications software packages written by DYSC.

The Series 500 is a highly modular system. Up to ten modules can be plugged into the basic unit according to the types and numbers of input and output signals. The total capacity is 272 analog inputs, 50 analog outputs, 160 digital inputs or outputs, and 160 channels of a-c or d-c power control. The maximum data input rate is 30,000 samples per second. The basic unit is priced at $2100, and individual modules begin at $250 each. The System 520, a so-called

ISAAC 2000

Control and data acquisition system for the IBM PC. [Source: Cyborg Corporation]

complete measurement and control system embodying six modules, is $4300. The system is user-programmable in an enhanced version of BASIC with about 40 special functions added. And the DYSC software is available.

Laboratory Technology Corporation got into the software business by a different route than any of the above companies. Last year at the Pittsburgh Conference, it exhibited a laboratory workstation computer, the Labtech 70, with a substantial number-crunching capability. This year it is offering the Real-Time Lab Notebook, a software package designed to run on the IBM PC.

Putnam, the founder and president of Laboratory Technology, says that over the last year features have become available on the PC that have advanced its power to the point where it is equivalent to the Labtech 70. Given the popularity of the PC and the storehouse of available software for it, it was pointless to try to compete head on. The strategy now is scientific software. A particular feature of the Lab Notebook is the incorporation of the popular 1-2-3 from Lotus Development Corporation. 1-2-3 is an example of one of the new waves in personal computing, integrated software. It combines electronic spreadsheet, data management, and graphics functions in one program.

In some respects, the Lab Notebook resembles the RS/1 "electronic notebook" of Bolt Beranek and Newman. However, it has real-time data acquisition capability and it runs on a personal computer rather than a minicomputer. Among the features of the Lab Notebook, in addition to data acquisition, are real-time control, data filing and management, data manipulation and analysis, statistical analysis, curve fitting, publication quality graphics, and technical report generation. The user can construct any procedure desired without having to resort to programming by means of menus whose items are selected by a mouse. The system also has "windows" that allow more than one item to be displayed on the video monitor at a time. One could simultaneously see a spectrum and a blown up portion of it, for example.

Cost of the basic Lab Notebook is $495. The user has to acquire 1-2-3 and a data acquisition and control interface separately.

Dapple Systems has eschewed the crowded field of chromatography. Dapple showed its Image Plus+ automatic image analysis system, which is based on the Apple II+ personal computer, and the Image Plus+ Model G, which uses an Apple IIe. Dennis Mayfield of Dapple says Apple is a natural choice because it is so popular. The target market comprises researchers with image analysis equipment who do not want to spend $60,000 or more to have an updated, automated version.

Prices from Dapple run from about $15,000 to $35,000 depending on the equipment needed. A full system for analyzing photographs or optical microscope images would include the Apple computer with video display and printer, a video camera, an interface card containing circuitry to connect the computer to the camera, and a video monitor for the camera. To analyze scanning electron microscope images, only the computer with display and printer and an interface card would be needed. The Model G includes a graphics tablet with a mouse for tracing or marking features on the image being analyzed.

The software allows the user to select features of the image of interest, measure the features on a digitized image,

and calculate parameters of the image, such as the mean distance between features or the number of features per unit volume. In addition, several statistical and graphical operations can be done.

Heyden & Son, Inc., a longtime publisher of scientific, technical, and medical texts, has broadened into the software business. The enterprise, new in January, is Heyden Datasystems. At the Pittsburgh Conference, Heyden exhibited its Spectrafile infrared spectroscopy data station built around the Apple IIe personal computer.

According to Nina Sammon of Heyden, Spectrafile is intended for the spectroscopist who has not yet automated his existing equipment. Choice of the Apple followed interviews with prospective customers that showed it to be most in demand. A feature of the software is a set of 21 spectroscopy-specific functions that the user can string together to construct a data acquisition and manipulation procedure. A single command, for example, tells the computer to search a spectrum library for one that matches an experimentally obtained spectrum. The user can also write and add to the program up to four functions to carry out any mathematical routine.

Cost of Spectrafile is about $6000, including the computer and interface device. Heyden also exhibited software for cataloging and retrieving information, an "electronic filing clerk." Priced at $75, Microfile could be used for such purposes as maintaining a library of scientific literature references.

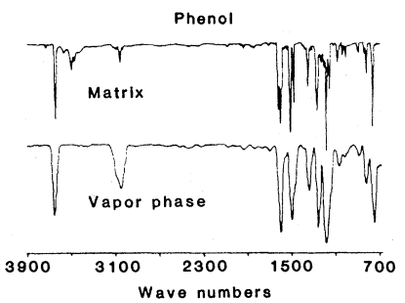
Another publisher, Elsevier Science Publishers B.V., is taking an altogether different tack to software. Extending its role as a publisher of science texts, Elsevier is publishing software written by outside scientists or authors. The main difference between book publishing and software publishing is that the software is not sold but licensed. Licensees must sign an agreement not to make more than four copies of the programs and not to distribute it to other users. The idea is not unique to Elsevier—other publishers have been marketing educational and medical software in a like manner—but it is new to the Pittsburgh Conference.

An Elsevier spokesperson explained that the company got into software publishing when it discovered its book authors were also writing software. The company's role is quite parallel to that in book publishing. It acquires programs from authors, turns them into "user-friendly" packages including a diskette and manual, and uses its marketing expertise to sell them. All software is refereed by two sets of third parties to guar-

Ultrahigh Sensitivity from GC-IR

A new technique that increases the sensitivity of gas chromatography–infrared spectroscopy (GC-IR) by three orders of magnitude was introduced at Atlantic City by Mattson Instruments, Inc. The key to the increased sensitivity is a new interface, called the Cryolect Matrix-Isolation interface, developed by Gerald Reedy and his colleagues at Argonne National Laboratory.

The heart of the device is a slowly rotating polished metal cylinder held at 12K within a vacuum chamber. About 1 percent argon is added to the carrier gas in the GC. After separation in the GC, part of the sample is split off to a detector for peak identification. The majority of the sample stream, however, is directed onto the surface



Sharper spectra

Sample molecules immobilized in a matrix produce sharper spectra.

of the cylinder where the argon and sample condense. The cylinder is then rotated 180° so that the sample is at the focal point of reflective IR optics.

In a conventional GC-IR interface, the IR spectrum is obtained while the sample is passing through a light tube. The investigator thus gets only one chance to obtain a spectrum, and typically only part of the sample is in the light tube at one time. With the Cryolect, virtually all of each peak is collected on the disk and the investigator can examine it at leisure—it remains intact as long as the cylinder is cooled. Sensitivity is thus higher; spectral quality is also improved because the transparent argon matrix prevents IR band broadening or shifting due to rotational absorption or intermolecular bonding.

In several papers presented at the meeting, Reedy and his colleagues reported that the technique could detect and identify samples in the picogram range, and that for many applications, GC-IR using the interface was actually more effective in identifying unknowns than was GC–mass spectroscopy. Unfortunately, the price of this sensitivity is high—about $104,000 for the interface alone.

—T.H.M.

A New Library for GC Unknowns

Gas chromatography (GC) is one of the most widely used techniques available for quantitative analysis. In the past, however, it was not very good for qualitative analysis because retention times and retention indices for a given compound could vary significantly from column to column, and often even for different runs on the same column.

That situation changed markedly in 1979 when Ray D. Dandenau and E. M. Zenner of the Hewlett-Packard Company reported on the use of flexible fused-silica capillary columns for GC. Retention times on these columns were highly reproducible from column to column (*Science*, 21 October 1983, p. 259). The new columns, combined with microprocessor control of GCs (which further increased reproducibility), made GC a realistic option for identification of unknown compounds.

Recognizing the utility of this new technology, Sadtler Research Laboratories—a company already well known for its spectral libraries—is bringing out the "Sadtler Gas Chromatography Standard Retention Index Library," a four-volume set containing data on 2000 compounds. Data for each compound are presented for four different columns. For the two bonded-phase columns, data are presented for four set temperatures and two temperature programs. For the nonbonded-phase columns, it is presented for five temperatures and two programs. In each case, aliphatic hydrocarbons are used as internal standards and the results are presented as both retention times and retention indices.

Sadtler plans to expand the index

antee it does what it is supposed to and that it is easy to use. The names of the authors and referees go with the software. A newsletter supplies licensees with updates as they become available.

All software is of the menu-driven type, so the user does not need to do any programming. At present, Elsevier offers six programs, some of them for the Apple II family and IBM PC personal computers and some for Hewlett-Packard or Digital Equipment Corporation desk-top or minicomputers. Eventually, all six will be available for the PC. And another six programs will be out by the end of the year. Prices range from $150 for a relatively simple statistics program that compares the similarity of different data sets to $1080 for a complex chemical education program that runs on a minicomputer.

Microsystems Research Corporation is not in the software business now but soon may be. At present, Microsystems Research manufactures plug-in boards for Apple II+ and IIe and IBM PC personal computers that allow the machines to control Mettler electronic balances. Called Softweigh, the plug-in for the Apple costs $349 and that for the PC goes for from $349 to $999 depending on how much, if any, memory is needed. Each unit can accommodate one or two balances, and no special interface adaptor or cable is needed.

However, Mark Goegelman, president of Microsystems Research, says he is looking at software for the future. Hardware is costly and there is the problem of maintaining inventories. Software built around standard hardware is a much better business. Another vote for the personal computer phenomenon.

Finally, the larger instrument manufacturers have not failed to recognize the allure of the personal computer. Some offered control or data systems for their instruments built around Apple or IBM machines. Allied Analytical Systems (a recent merger of the Jarrell-Ash division of Fisher Scientific and the Analytical Instrument division of Instrumentation Laboratory) showed inductively coupled plasma atomic spectrometers with Apple IIe or IBM PC/XT personal computers. "People like both," said an Allied salesperson.

In the spectrophotometer area, Bausch & Lomb advertised applications software for its Spectronic 1001 and 2000 instruments written for the Apple IIe. Software for the IBM PC and for the Hewlett-Packard 150 will soon be available. And Beckman Instruments announced interfaces to connect its DU-6 and DU-7 spectrophotometers to all models of the Apple II and to the IBM PC. Finally, the Oriel Corporation, which manufactures modular instrumentation for spectroscopy, offered Apple systems for computer control of fluorescence and absorption instruments.

Where will it all end? One interesting test would be to watch the Perkin-Elmer Corporation. Perkin-Elmer's president Horace McDonell, Jr., extolled to the press the virtues of transportability of software between different types of computers and the ability to control instruments from different manufacturers with one computer. Adherence to industry-adopted standards was cited as one way to move in this direction. Perkin-Elmer also has developed an immense quantity of applications software for the instruments it manufactures, designed to run on the company's own professional laboratory and superminicomputers, which at present are not compatible with the Apple or IBM PC. Will it ever be possible to run Perkin-Elmer software on these machines?—**ARTHUR L. ROBINSON**

Technical Publishing Workstation

Each year, the Pittsburgh Conference seems to come up with one or more products that are just plain fun to play with and more than a little useful as well. A candidate this year comes from Demonics Limited. Demonics showed for the first time its technical publishing system, comprising a computerized workstation for laying out the pages of a document and a laser printer for its production.

The workstation is built around a Motorola 68000 microprocessor. Current software possesses only rudimentary text-editing capabilities, so most users would probably feed in text via an interface to an outside computer with word processing capability. What the workstation does is lay out the text in a variety of type styles and sizes and in a format specified by the operator. The video monitor screen allows display of type as small as 6 point. (This article is set in 9 point.)

Publishing system

The 1320 × 1320 line resolution screen displays an image of the page exactly as it will look when printed. [Source: Demonics Limited]

Photographs, drawings, and other visual material can enter the system in two ways. A "frame grabber" can digitize television camera or video recorder images, or a digitizer can scan the artwork. Resolution is 120 pixels per inch with 64 shades of gray.

While viewing the material on the video monitor, the operator can blow up or reduce the size of the artwork, can crop it to eliminate unwanted features, and can "electronically airbrush" it to remove blemishes or add artifacts. The material is then placed on the page and the existing text moves on the page to accommodate it. Figure captions are also incorporated.

Operation is largely menu-driven, which is to say that the operator need only choose from among options displayed on the video monitor during the document preparation. Selection of items on the menu and manipulation of objects on the monitor screen (photographs being cropped, for example) is by a mouse, although there is also a keyboard console.

A 144-megabyte hard disk memory can store more than 1000 document pages. The laser printer can run off documents at the rate of 300 or 600 pages per hour.

The basic system comprising workstation and printer is priced at $59,500. Cameras and digitizers are available from Demonics or can be user supplied.—**A.L.R.**