of only about 1 part in 1000. The FT-ICR spectrometer, in contrast, can produce a spectrum with a resolution of 1 part in 20,000 or 30,000—good enough for elemental analysis—in less than 200 milliseconds. Wilkins and Michael L. Gross are now developing a prototype interface to connect the gas chromatograph to the instrument.

There are apparently only three FT-ICR spectrometers in existence. Comisarow has one that he has constructed himself, Nicolet has a prototype commercial instrument, and Wilkins and Gross have one that is almost finished. The Nicolet people have been promising for at least a year that their instrument will be on the market soon, but they have had problems obtaining what they consider to be satisfactory relative peak intensities (that is, if there are 9 parts of an isotope with mass 91 and 1 part with mass 92, the relative peak intensities should be 9 to 1). Wilkins suggests that this problem may result both from cell design and from the fact that the ions are out of phase with each other since they are not excited simultaneously. Nicolet hopes to solve the problem, but may bring the instrument out soon anyway. Nicolet president Jerry Holcombe says that the instrument will probably be available to customers this summer. The selling price is expected to be about $150,000, which compares favorably with the $400,000 cost of a conventional ultrahigh-resolution instrument.

Many people may not need to wait for a commercial instrument, however. There are now available a large number of used nuclear magnetic resonance spectrometers in which the magnets do not produce fields sufficiently homogeneous for high resolution. Because of differences between the two techniques, however, these magnets still have more than enough homogeneity for FT-ICR. Anyone with a reasonable knowledge of electronics and Fourier transform technology should thus be able to construct his own spectrometer at relatively little expense.

Before too many people plunge into the field, however, it will be necessary for the potential of FT-ICR to be demonstrated in practice. That is what the three active groups are doing now. Wilkins and Gross, for example, are planning to compare spectrums obtained on their instrument with those obtained on an ultrahigh-resolution MS-5076 spectrometer produced by AEI Scientific Apparatus. In this way, they hope to provide benchmarks to show precisely how good the technique is. The other investigators are using different approaches to accomplish the same end. The experiments to date have been only prototypes which serve to indicate some of the features of the FT-ICR method, but the results are encouraging and of sufficient interest to warrant further application of the technique.

—THOMAS H. MAUGH II

# Smart Instruments: Microprocessors Not the Whole Story

One evident characteristic of the Pittsburgh Conference was the spate of new products either introduced or not previously shown at the laboratory equipment exposition. Many of the new instruments were equipped with microprocessors; it would not be much of an exaggeration to say that every other booth prominently featured microprocessor-controlled apparatuses of an astounding variety. At the same time, it was abundantly clear that these ultraminiature processor units were far from the whole laboratory computer story. For the most part, data-handling applications and laboratory automation systems continue to require programmable calculators or minicomputers. Some of the minicomputer data systems exhibited were, however, actually built around one or more microprocessors.

Microprocessors are programmable integrated circuits on one or a few silicon chips and are the equivalent of the central processor unit of a computer. Because they pack so much computing power into such a small space for, in many cases, only a few dollars, these circuits have been hailed as the devices that will make the "electronics revolution" really take off. Intelligent instruments for laboratory use that can control and monitor their own operation and log and manipulate the data they produce are expected to be one manifestation of this revolution.

What probably characterizes the progress made by microprocessors in instrumentation this year is that they are no longer confined to the top-of-the-line Cadillac models. Embracing this trend wholeheartedly is the family of instruments shown by the Perkin-Elmer Corporation, Norwalk, Connecticut. Perkin-Elmer introduced 20 new instruments at the 1977 Pittsburgh Conference, and 12 of them incorporate microprocessors to handle various aspects of instrument control or data reduction. For example, the company exhibited three new atomic absorption spectrophotometers that span the low-to-medium price-performance range (base price from $6000 to $9000), and all are microprocessor-controlled. It is, said a Perkin-Elmer spokesman, still possible to buy an atomic absorption apparatus without a microprocessor, but no one from the company will show one unless specifically asked.

The number and variety of microprocessor-equipped instruments at the Pittsburgh Conference was far too great to permit even listing them all. The following three examples may, however, indicate the ways manufacturers are using the tiny computing chips.

The Varian Instrument Division, Palo Alto, California, displayed two atomic absorption spectrophotometers equipped with the "computer on a chip." The top-of-the-line model, a double-beam instrument, incorporates all digital circuitry, a feature that reduces instrumental sensitivity to external sources of electrical noise. A microprocessor-like preprogrammed circuit, operated by way of a keyboard, is used to enter the flame setting desired, to monitor the gas-flow system, and to shut down the instrument in emergencies. A second microprocessor, operated from a separate keyboard, can do some kinds of data handling, such as reporting concentrations, peak heights, peak areas, and the mean value of a series of measurements. An optional automatic sample dispenser permits automated injection of up to 25 different samples in succession. The price of the spectrophotometer ranges from $9,600 to $12,900, depending on the options selected.

Not all instrument settings are by way of the microprocessors; certain parameters which are not changed often, such as lamp brightness, must be entered via rotary switches. This necessity precludes total automation because a remote computer cannot physically turn switches. A Varian spokesman says it would be too expensive to completely automate the spectrophotometer. The company also exhibited a lower-priced ($6600 base price) instrument that uses one microprocessor to control the gas and flame operation only.

Orion Research Inc., Cambridge, Massachusetts, introduced a digital specific ion meter controlled by a microprocessor. The meter uses three types of electrodes: $pH$, specific ion, and gas-sensing. Analytical parameters are entered via digital switches on the instrument's control panel; standardization and blank correction are accomplished by way of push buttons. No calibration curves, tables, or calculations are required of the operator, as the microprocessor is preprogrammed to solve the electrode equations using the parameters entered by the operator. Concentration, $pH$, or millivolt values are determined by direct or indirect methods selected by the operator using front panel controls and appear on a digital display. Cost of the meter is $1595.

Baseline Industries, Inc., Lyons, Colorado, demonstrated a microprocessor-controlled portable gas chromatograph weighing about 20 pounds. Control com-

# Instrument Highlights

## Coping with the High Cost of Instruments

One of the most important problems confronting investigators in biology and chemistry today, according to Richard N. Zare of Columbia University and John D. Roberts of the California Institute of Technology, is the increasing sophistication, size, and price of major instrumentation. Many types of instruments and their associated computers for data acquisition and analysis now cost in excess of $250,000 and may eventually reach $1 million. The performance of these instruments, Zare and Roberts argue, is often orders of magnitude ahead of their immediate predecessors, and they offer unusual opportunities for major breakthroughs in many areas of research. But the growing price of the instruments is straining the budgets of universities and funding agencies and threatens to consume all the funds that are available for research.

The magnitude of the problem is illustrated by a recent informal spot-check conducted by the National Science Foundation in chemistry departments representative of some 50 major universities. The survey shows that these departments have an average of about $3 million invested in instruments, and some have as much as $6 million. Furthermore, the operation and maintenance of these instruments cost the departments an average of about $500,000 per year, apart from the cost of water and electricity—which in some cases is as high as $150,000.

Major instruments generally have a useful life of about 8 years. The departments thus have to spend 12 percent of their investment, about $360,000 per year, simply to stay even. And to have all the instruments that would be useful to the chemists, the departments estimate, would require an additional investment of from $350,000 to $2.7 million. These figures are only for chemistry departments. When the capital investments of biology, physics, and other departments are added in—not to mention those of medical schools, private and government institutions, and the like—the total cost becomes staggering.

To explore ways of meeting some of these needs, the National Academy of Sciences has formed a panel to assess instrumentation needs in chemistry, biochemistry, and biophysics. The panel is chaired by Frank Bovey of Bell Laboratories and Elkan R. Blout of the Harvard Medical School. It will examine current funding policies, the effectiveness with which current major instrumentation needs are being met, and anticipated future instrument developments and needs. The panel is also expected to formulate recommendations for future funding policies and priorities.

One important aspect of the study, Roberts says, should be the consideration of new ways to use instruments. These might range from the operation of an instrument service center to the formation of research centers in each special subdiscipline. These options would cause a profound change in the "sociology" of chemists, whom Roberts characterizes as rugged individualists, each with his own laboratory and complement of instruments. In the past, Roberts says, this individualism has served the discipline well. But as chemical research demands the use of increasingly sophisticated instrumentation, this type of independence will become increasingly untenable. It will then be necessary to investigate methods of operation that involve a great deal more collaboration among individual scientists.

—T.H.M.

## Instrument Shortage Slows Brazilian Science

*São Paulo.* The importance of instrumentation to modern scientific research is being illustrated anew here in Brazil, where a growing shortage of replacement parts and new instruments is substantially slowing the pace of research. The shortage stems from the fact that Brazil has only a small indigenous instrument industry; most major pieces of equipment found in university or government laboratories come from the United States or Germany. A ban on nonessential imports imposed by the Brazilian government in the past 2 years has severely restricted that supply link. Even when a researcher is able to win an import license from the government, the procedures are complicated and can take up to 2 years, during which vital equipment must sometimes lie idle or experiments must be postponed. "The import limit is hurting research very seriously now," says Ernesto Giesbrecht, director of the large Institute of Chemistry at the University of São Paulo.

The import restrictions began in the wake of the sharp increases in international oil prices several years ago. Because Brazil imports most of its oil, it was rapidly faced with a balance of payments deficit large enough to worry many foreign banks and credit agencies, which put pressure on the Brazilian government. Under the restrictions, most imports other than oil are either forbidden or assessed a duty equal to 100 percent of their value, unless a government permit can be obtained.

The National Research Council (known by its initials CNPq) is supposed to help scientists cope with the situation, since it has authority to obtain permits for anything necessary for the country's research effort. But the amount of red tape required is such that many universities have resorted to hiring special counsels or "fixers" just to cope with the bureaucracy that has arisen to administer the import permit program. Most scientists seem convinced that the system is unworkable.

Officials of the CNPq defend the import restrictions and have tended to minimize their impact. They admit that there have been substantial delays and many complaints, but attribute part of them to scientists' lack of familiarity with the system. CNPq President Jose Dion de Melo Telles told *Science* that his agency stands ready to respond to specific needs wherever it can be documented that research is mands for entry and retrieval of all data are by way of the seemingly ubiquitous Touch-tone type keyboard. Up to 16 commands (or 100 in a more expensive version) to control operation of the chromatograph are also entered in this manner and stored in the machine. A strip-chart recorder displays the chromatogram, but an optional plug-in circuit card provides the ability to do operations such as peak integration, peak height determination, and baseline correction. The basic 16-step instrument is priced at $3850. The version with 100-step control, flame ionization and thermal conductivity detectors, and integrator card costs $5800.

Exactly how much capability the use of microprocessors adds to these and the many other instruments on which they are appearing is not always easy to dis-



being seriously hurt. "We are deeply concerned about this problem," he said.

In any case, the effects are strikingly evident to a visitor at Brazilian research installations. They are perhaps most evident in chemistry laboratories, such as those at the São Paulo Institute, which depend increasingly on sophisticated instrumentation for a wide range of investigations. Chemists find themselves ordering equipment and supplies in greater abundance than they normally would, hoping that when they arrive 1 to 2 years from now, they will be what is actually needed for experiments often not yet conceived of in detail.

Elsewhere, too, the shortages are evident. At a remote sensing laboratory attached to the Brazilian space agency, an expensive multispectral camera sits waiting for a new cathode-ray tube to replace one that burned out months ago; lack of the camera has hindered fully effective use of a $700,000 image analysis system. Researchers at a solar energy institute painstakingly built their own electrolyzer to produce hydrogen rather than delay their research program for the year and a half that it was estimated an imported model would take to acquire. And the new director of a graduate engineering center at the University of Rio de Janeiro says that the lack of spare parts and new instruments is hurting his program so much that he plans to start several instrumentation groups within the university.

Several scientists say that university research groups have taken to juggling their accounting, ordering instruments or equipment for which they do not yet have funds but expect to in next year's grant, in an effort to keep the flow coming in. Most are simply planning their experiments with greater care and thinking farther ahead. That in itself could be considered a beneficial effect of the import restrictions. The overall impact, however, is clearly slowing down the Brazilian scientific enterprise.—ALLEN L. HAMMOND

## Photoacoustic Spectroscopy Comes of Age

In the hullabaloo that surrounds the Exposition of Modern Laboratory Equipment at the Pittsburgh Conference, it often seems to be forgotten that nearly 500 papers on instrumental techniques are presented. These papers generally provide a good indication of the kinds of instrumental techniques that are just over the horizon. A case in point is photoacoustic spectroscopy. Two years ago at the Pittsburgh Conference, Allan Rosencwaig of Bell Laboratories presented one of the first in a recent series of papers describing the use of photoacoustic spectroscopy on solids (*Science*, 4 April 1975, p. 38). This year, two instrument companies exhibited for the first time commercial photoacoustic spectrometers specifically designed for that purpose.

Photoacoustic spectroscopy is an unusual technique. The sample to be studied is placed in a specially designed airtight cell equipped with a sensitive microphone and exposed to intermittent (chopped) monochromatic light. If the sample absorbs at the wavelength of the incident light, the light energy is converted to heat energy, and the temperature at the surface of the sample fluctuates at the chopping frequency of the light. This temperature fluctuation, in turn, creates a pressure fluctuation in the air in the cell; the fluctuation is detected by the microphone and converted to an electronic signal. If the wavelength of the incident light is varied, it is possible to obtain a complete absorption spectrum of the sample.

The acoustic response does not depend on reflected or transmitted light and, thus, does not depend on the physical state of the sample. More important, it has the advantage of not being very much affected by light scattering, which is one of the most serious problems associated with conventional spectroscopy of solids. The technique is thus suitable for use on various materials, including powders, crystals, gels, smears, and even intact biological samples. One example of the many potential uses of the technique is the determination of the spectrums of compounds adsorbed onto the surface of thin-layer chromatography plates.

The two photoacoustic spectrometers introduced at the conference were developed by Rosencwaig, who is now with Gilford Instrument Laboratories of Oberlin, Ohio, and by Donald M. Munroe and Harry S. Reichard of Princeton Applied Research Corporation, Princeton, New Jersey. It is difficult to compare the two instruments, but representatives of the two companies agree that some generalizations can be made. The Gilford instrument is a double-beam spectrometer with two sample cells, while the Princeton instrument contains only one. The Gilford instrument can thus compare two slightly different samples directly, while the Princeton instrument requires an optional accessory to store the spectrum of one sample for comparison with a second. The Princeton instrument does produce a source-compensated spectrum when performing such difference spectroscopy, however. The Princeton spectrometer is equipped with an electromechanical chopper, whereas incident light in the Guilford instrument is modulated electronically. Electronic modulation is more flexible, but electromechanical chopping permits more light to reach the sample.

The Princeton spectrometer seems to have better electronics and is able to scan faster because of a better signal-to-noise ratio. It also seems to have a better designed instrument package that includes a built-in X-Y recorder. Both instruments cost less than $30,000, and both companies promise delivery within 6 months.

Some investigators who are skilled in electronics have already constructed their own photoacoustic spectrometers and have begun to explore some of the potential uses of the new technique. But the appearance of a commercial instrument will make the spectrometer available to a greater number of individuals. And as judged by the great interest of those attending the Pittsburgh Conference, applications of the technique should flourish during the next few years.—T.H.M.

cern. As one seasoned observer of the Pittsburgh Conference wondered rhetorically, "Microprocessors on instruments are like Touch-tone telephones; they're nice, but do they really improve the fidelity of communication between here and Washington?" More than one sales representative on the floor of the exhibition hall admitted that in some cases little more was involved than replacing knobs with a keyboard. Another suggested that the manufacturers like microprocessors because the reduced labor costs make instruments cheaper to build, as much as for any other reason.

Whatever the answer to this question, it is clear that in most cases anything beyond rudimentary data-handling tasks requires more computing power than the present generation of microprocessors can muster, or at least more than instrument makers are drawing from them. Microcomputers constructed around microprocessors and possessing considerable computer power were shown at the instrument show, for example. Still, the limitations of microprocessors seemed evident. If every other booth displayed instruments containing these wonder circuits, many of the same booths also displayed data systems based on minicomputers.

A computer-controlled titration system shown by the Mettler Instrument Corporation, Princeton, New Jersey, illustrates one occasion in which a microprocessor alone is not enough. The titration system is built around four titration heads and 20 burettes, giving a total of 80 possible wet chemistry procedures, and is capable of carrying out 120 titrations in an 8-hour period with no operator present. Since each of the samples may require a different analytical procedure, programs for the titrations are stored in a desktop calculator. There are no knobs anywhere on the instrument, whose operation is initiated through the calculator. Control of the titrator itself is by way of a microprocessor within the instrument, but the microprocessor receives all its instruction from the calculator. The titration system costs from $55,000 to $75,000.

If storing all the instructions needed for fully automated operation requires more than a microprocessor, so does storing all the data accumulated during a run for further manipulation. It may, however, be simply a matter of more fully utilizing the microprocessor by making a full-fledged microcomputer. The Princeton Applied Research Corporation, Princeton, New Jersey, has taken this approach with its newest optical multichannel analyzer system. An optical multichannel analyzer is essentially an electronic spectrograph for recording the spectrum of almost any optical experiment. A monochromator disperses the light it receives, but rather than being scanned past a slit and into a detector, the entire spectrum is detected simultaneously on a large-area detector. Thus, data can be collected much more rapidly than normally. Princeton Applied Research uses an integrated circuit array of silicon diodes in its detector, which operates similarly to a television camera tube (vidicon). The control console for the system contains a microcomputer, and a flexible disk for mass storage. Spectrums from several hundred runs can be recorded and stored for subsequent calculations. Spectrums are displayed on a cathode-ray tube display in the console, which can operate up to four analyzers at once. Cost of such a system varies from $22,000 to $27,000.

### Micro-, Small, and Minicomputers

Many computer companies exhibited somewhat similar data handling systems under the general term *small computer*. These systems often consist of some combination of a microcomputer; a keyboard terminal and a cathode-ray tube display integrated into one unit; a printer; a plotter; and mass storage devices such as tape cassettes or flexible disks. A small computer system of this type made by the Digital Equipment Corporation, Maynard, Massachusetts, sells for $11,000 to $20,000, depending on options.

The minicomputer data systems offered by instrument manufacturers for almost every conceivable spectroscopic technique have as their selling point the software—the programs needed for running the computer—which can take several man-years of effort to develop on one's own. This can be a powerful motivation for buying from the instrument maker rather than from the minicomputer manufacturer.

Manufacturers of computers, or those who assemble computer systems from hardware they buy, can counter this argument by developing and selling their own programs along with their computers. Computer Inquiry Systems, Englewood Cliffs, New Jersey, for example, uses a Hewlett-Packard minicomputer as the basis for its automated laboratory system. The company does not sell instruments itself but claims a superior performance for its data system, which can be used with a variety of types of instruments because of a specially designed interface circuit called a Digimetry coupler and because of its better program package. The user can also write his own Fortran programs to run on the system.

Like the majority of laboratory data systems displayed at the conference, it is capable of handling several instruments at once (as many as 60) and can interact with several (as many as 8) remote terminals. The system can also simultaneously be acquiring data while it is processing previously acquired data or executing programs written by the user. It also resembles the majority of data systems exhibited in that it is only suitable for relatively "slow" experiments, such as chromatography, optical absorption, and fluorescence. "Fast" experiments, such as mass spectrometry, Fourier-transform infrared spectroscopy, and Fourier-transform nuclear magnetic resonance, require their own dedicated computer. The price for the Computer Inquiry data system begins at $42,000, which includes the computer, a disk for mass storage, a keyboard–cathode-ray tube terminal, one Digimetry coupler, and the software.

Another company, Nuclear Data, Inc., Schaumburg, Illinois, is one of many that make minicomputer-based data systems which can handle fast experiments that accumulate data at a rate exceeding about 100 digital bits of information per second. The Nuclear Data computer is unique, however, in its concept, which involves one of the current buzzwords—distributed processing—and four microcomputers. One microcomputer operates as the central processor unit of the entire system. As many as three other microcomputers act independently to control data acquisition and display subsystems. Interaction between the microcomputers is by way of a high-speed communications channel of a novel design, which the company calls a Combus. Combus allows components of the system to begin communicating before previously begun interactions between other components have been completed, thus speeding up operation considerably. The price is comparable to that of other data systems, starting at $34,700, which includes one dual flexible disk and one keyboard–cathode-ray tube terminal. At present, applications programs for gamma and x-ray spectroscopy, ESCA (electron spectroscopy for chemical analysis), and neutron activation analysis are available.

One theme that reappeared throughout the exhibition was the need to make computerized instrumentation seem "friendly" to analytical chemists unfamiliar with computer technology. Hewlett-Packard, Palo Alto, California, displayed two gas chromatograph–mass spectrometer instruments that were adorned with computerized data systems. The company seems to distinguish between two groups of users. The first includes those with pri-

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marily a chromatography background, but who want to take advantage of the extra information provided when a mass spectrometer analyzes the chromatograph peaks. For this class of customer, a system employing a programmable calculator for data handling is recommended. Not only is it less expensive (below $50,000), but the calculator with its typewriter-like keyboard seems less intimidating than a minicomputer. For the scientist experienced in mass spectrometry, a more sophisticated system employing a minicomputer for simultaneous data handling and acquisition is encouraged. The cost, accordingly, is much higher—about $121,000.

A major problem with computers has always been, having an experimental apparatus and a computer, how does one hook them together? One answer beyond home- or custom-made interfacing circuits, and thus an answer that makes computers seem "friendlier," was displayed by IBM. Called a Device Coupler, this all-purpose interface enables users to start running experiments in days, not the customary months, IBM claims. The coupler can receive either analog or digital input signals from several instruments and can send out either analog or digital information for instrument control or for further processing or display by other devices. The coupler can be used in a variety of configurations; it can be the interface between a computer, the instrument, and a terminal, or some combination of these. It can also be used with programmable calculators. The coupler is derived from a similar instrument designed for IBM scientists for use in their laboratories. Prices begin at $3050 and go up as plug-in modules are added.

Perhaps the friendliest of all worlds would be the one in which a laboratory manager hires out the task of automating his laboratory to an outside company, which then takes care of every aspect of the job from planning to turning over a finished, ready-to-run operation. There were companies at the Pittsburgh Conference selling exactly this service. One such organization, Codevintec Pacific, Inc., Woodland Hills, California, was ready to computerize anything from a single instrument up to a full laboratory. A spokesman for the company claimed that many people were sufficiently intimidated by their lack of expertise and by the cost of having to develop interface circuitry and software that it was worth it to them to pay for a finished system.

—ARTHUR L. ROBINSON