

grams in their memories; the user simply selects the program of interest—spectral overlay, for example then changes the preset parameters as needed

For routine scanning and other operations in which printed spectra are not usually required, VDTs can serve as alternatives to costly printers or chart recorders; if hard copy is needed, notes Sequera, the operator performs a "video dump," in which the screen image is transmitted electronically to the printer. "The only drawback is a possible loss of resolution," says Sequera, "since the printer records only what's on the display. Resolution is thus limited to that of the screen, which may not be very high." (Several manufacturers claim to solve that problem with a 16-bit resolution feature, in which the data is sent to the printer from the microprocessor rather than from the VDT screen.)

It's debatable, however, that a video display is needed in quality control or other repetitive tasks, says Kontron's Wagener. Moreover, such devices could needlessly complicate instrument operation, thus calling for more experienced lab personnel.

• Data-management. The advent of the personal computer (PC) and microelectronics during the past decade has generated the most dramatic changes in spectrophotometry. Although most instruments feature selfcontained minicomputers preprogrammed for the most common procedures, customized software and the ability to tie the spectrophotometer to a PC via bit parallel or bit serial interfaces has greatly enhanced data manipulation and storage (especially if a high-capacity hard disk system is used). But while such bells and whistles greatly boost the spectrophotometer's performance, they also drive up the price; as with any purchase decision, the thoughtful spectroscopist must decide how often such options will really be needed, and whether usage will justify the cost.

If the answer is "yes," there's a veritable software smorgasbord to choose from. For example, Beckman, Gilford, and several others offer software for unattended or highly automated spectrophotometry, thus reducing time and tedium in repetitive, single-variable tasks. Programs are also available for such routine tasks as calculating the area under peaks, overlaying scans obtained from different labs on a single screen, smoothing and interpolation, archiving of spectra and other data ("a must if you're working with patentable products or processes," says one spectroscopist), storage of standard spectra for comparison against unknown samples, and word-processing for customized report preparation.

Other programs, such as Beckman's DU Data Leader, allow the operator to display data from several samples in a colorful three-dimensional format. A recent Varian technical report (No. UV-39, December 1986) details yet another example: the off-line use of an IBM PC/AT and a commercial telecommunications program known as Kermit to retrieve and manipulate archived spectral

data, then report the results via the Lotus 1-2-3 spreadsheet package.

Although every manufacturer boasts "user-friendly" operation, some sources note that—as with VDTs—even relatively simple computerized instruments may complicate operation, and thus boost costs by requiring relatively skilled personnel to operate them. "The best approach is to select the simplest model that will serve your needs, but one that can also be easily upgraded in the future," says G.E.'s Williams.

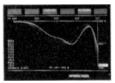
SPECTROPHOTOMETERS



Grating spectrometer. The 340E 0.34-meter grating spectrometer is the latest addition to the line of light measuring instruments available from Spex Industries (Edison.

NJ). Longer focal length increases wavelength dispersion at the exit plane by 50 percent, and allows additional room, making it possible for the 340E to accept swingaway mirrors on optional dual entrance and exit ports. Two detectors (such as multichannel arrays and photomultipliers) and two radiation sources may be attached and accessed easily. Kinematic mounts permit quick grating changes, and compatibility with a range of Spex accessories and data control systems.

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UV/Vis spectrophotometer. The Kontron Uvikon 860 ultraviolet-visible spectrophotometer from Kontron AG (Zurich, Switzerland) uses its large curve memory and sophisticated post-measurement calculation facilities to allow many sample comparisons to be made at once. As many as 12 curves can be superimposed on the video display. Highlighting of individual curves and scale expansion make detailed comparisons easy. Curves may be added and subtracted, to check effects of different background absorbancies. These calculated curves can then be stored in the system's memory, for later recall and comparison, which may be plotted, including highlighting, for permanent records.

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A variable long pathlength gas cell from Spectra-Tech (Stamford, CT) has been developed to provide the advantages of gas and vapor analysis with FTIR spectrometers. Able to determine components in gas or vapor mixtures from the percent level down to parts-per-billion, the gas cell can help in analysis of chemical process streams; in monitoring toxic gases; in the measurement of contaminants of components in breathing gases; and in analysis of compressed and bottled gases. Custom-designed interfacing optics allow easy use on all FTIR spectrometers; cast aluminum design assures safe operation to 150 psi or under vacuum, with operating temperatures to 150°C.

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Colorimeter. The u-Colorimeter from Whatman (Kent, U.K.) enables the absorbance or concentration of samples to be read directly from microcuvette strips. Using microprocessor technology, the u-Colorimeter employs two controls in conjuction with the IC display to guide the user through the measurements. As many as 12 wells can be measured and the results downloaded to a personal computer or printer using an RS232 interface. The u-Colorimeter uses interchangeable interference filters available within the wavelength range 400-700 nm.

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