The
SPEX
Speaker

# SCAMP DEFIES
THE DATA CRISIS

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Of all the world's wide-scattered resources, information is one of the most valuable. Yet even as volume after abstracted volume of publications go gushing on around us, it seems that hard, conclusive data is rapidly becoming as scarce a quantity as gas or oil. Old reserves threaten to evaporate without warning, so you find yourself spending longer and longer hours in the lab, often working as fast as you can just to stay even. Where once a single spectrum or chromatogram used to be enough, you now have to run three or four. Each experiment multiplies, burning up your precious time as you try to sort through peaks or background, and every question answered leads to two more unsettled. You dig deeper, try different techniques, consider more efficient equipment — anything to squeeze a little more mileage out of your data. You know the well isn't dry. Not by a long shot. There's still plenty of crude down there waiting to be tapped. All you need is a way to pump it out, a place to store it, something to refine it into a finished, high-octane product.

It's not a new problem, though as with any analytical bottleneck it only gets worse the longer it goes unchallenged. Because of that, potent and specialized instruments are constantly being mustered for fresh assaults — multichannel analyzers, scalers, mini- and macro-computers — a plethora of hardware with such an insatiable appetite for software that data accumulation and reduction often have to take a back seat while the processing becomes an end in itself. Then another crisis intervenes as the only true nonrenewable resource dries up — your time.

So it was that SCAMP was created, to meet the demands of instruments from Atomic Absorption to Stress Analysis, from Thermogravimetry to X-ray Fluorescence, with interfacing as un-

complicated as a BNC cable, with processing, presentation, and output of data as simple as a single push of a button. Since there's no computer vernacular to master, you begin your experiments as soon as the SPEX SCAMP data system is out of its crate. And once introduced to your instrument, SCAMP extracts the essentials and hands them over to you automatically in a complete, report-ready form. Equally important, SCAMP interacts with the unique environment of your lab. It isn't dedicated, so you, rather than the machine design, decide what information is really important.
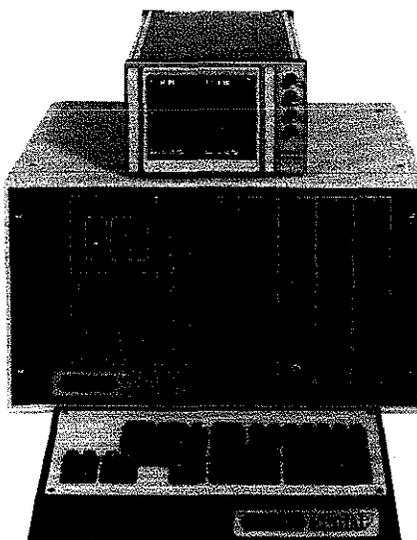
One Signal or Four?

SCAMP is not biased in favor of any particular discipline or equipment, whether it's a commercial device or one of a kind, as long as the data is in the form of Binary-Coded Decimal (BCD) or common analog output which falls, naturally or with attenuation, between 0 and 100 mV. SCAMP will accept up to four of these inputs into a memory array of 4096 sample points (with a precision of 1 part in 4096). Displayed on a high resolution CRT, the data can be divided into halves (2048 points) or quadrants (1024). This allows for double-beaming, ratioing, and even monitoring different instruments at the same time. The last feature, for instance, would let you simultaneously record a thermogram during decomposition of a sample while identifying the out gases with Raman Scattering [1]. The particular value of multiple inputs is emphasized in Fig 1, a Differential Thermal Analysis (DTA) of hydrated copper sulfate. Trace A is the difference between the temperature of the sample and an inert reference material as the two are heated in a chamber whose temperature, Trace B, is monitored as a function of time. SCAMP keeps track of both signals. Note that the rise in DTA chamber temperature is not linear and, therefore, the relevant parameters, such as peak position and area, would give erroneous results were not the axis rescaled as a true function of temperature as in Trace C. Here the vertical axis remains differential temperature, while the horizontal becomes temperature. On SCAMP, as we'll see, a single keystroke command is enough to accomplish the entire rescaling and consequent cross correlation.

The sampling rate of data acquisition can be controlled internally by SCAMP's own clock, data points being recorded at intervals from 0.1 to 20 seconds. Alternatively, an outside trigger can be con-
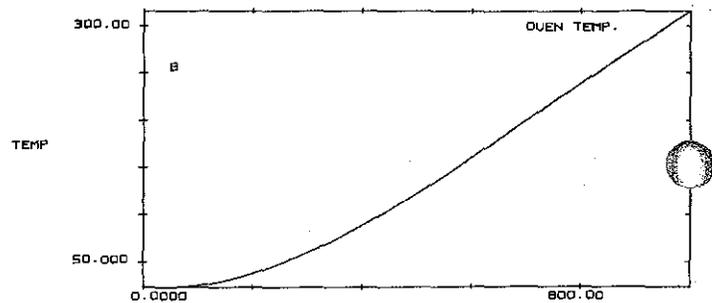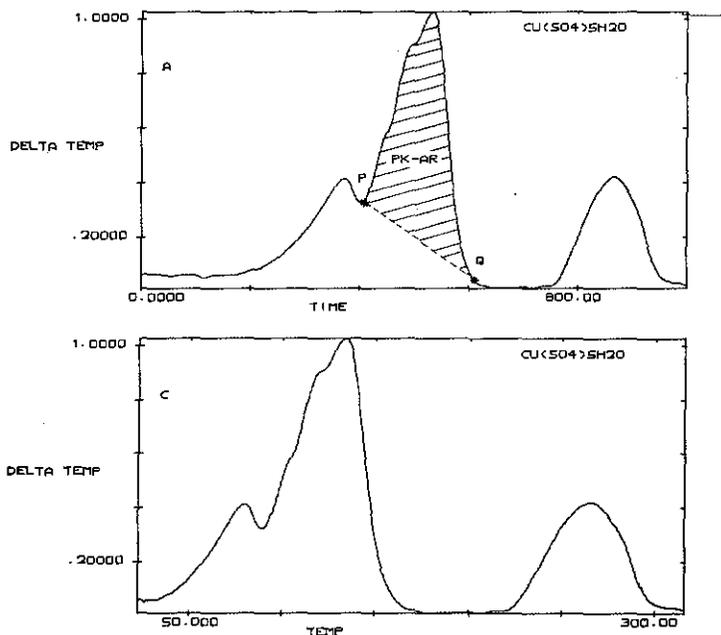
Figure 1 Differential Temperature (between reference and sample) and the temperature of the chamber from a DTA were recorded simultaneously by SCAMP as a function of time. Note the non-linear rise of temperature that's especially evident at the start of the experiment. The true DTA data is found by displaying trace A versus trace B, as seen in C.

We've also shaded A to show the result of calculating the peak area (PK-AR).

nected so the signal is sampled only on demand, when it is ready. With our DPC2 Digital Photometer, for instance, this means data can be taken after a selected number of counts have reached a reference detector. (Data acquisiton on the SCAMP can also be extended to 100 MHz with a waveform recorder [2].)

In its SCAN mode, SCAMP drives a stepper motor through a user-defined region and so it's compatible with all our spectrometers. Yet a simple counter circuit can convert SCAMP's pulse output to a ramp voltage such as those that drive many Nuclear Magnetic Resonance (NMR) or Electron Paramagnetic Resonance (EPR) devices. As we'll see, combining this hardware interaction with SCAMP's keystroke-linking memory frees your attention for other work. SCAMP may signal average over a sample spectrum, for instance, subtract away a solvent blank, and have a completely annotated plot waiting for your approval when you return.

Memory on Display

The real distance between your instrument's output and the final result, be it a go/no-go value for quality control, an impurity concentration, or a chart of the relaxation modulus of polystyrene, is more than just a few meters of BNC or BCD cable. Even from the start of this journey from raw signal to hard fact, SCAMP keeps the data right in front of your eyes on a high-resolution CRT where it can be monitored and instantly expanded horizontally or vertically to locate those subtle changes that make all the difference between success and rerunning the experiment. In Fig 2 the upper and lower CRT traces are exactly the same spectrum except that the peak is barely discernable — until expansion

is invoked. And since each trace has its own vertical control for independent positioning on the screen, spectra are easily overlaid for ultra-fine comparisons.

Two mobile cursors (P and Q, the bright dots on the screen) lend added precision to these examinations as well as let the operator interact directly with the data because located on the bottom of the CRT is a set of coordinates listing the cursor positions and vertical magnitude or intensities. One coordinate shows the location of the cursor in SCAMP's memory (0 to 4095), while H defines a horizontal position that may be scaled to any units such as nanometers, degrees, parsecs, or percent depending on your application. (This scaling is done automatically in the SCAN mode.) In Fig 2, P is at 394.20 nm. The V cursor coordinate is the amplitude or intensity of the particular data point (200.70 pps for P). Both these H and V values of the cursors (or their differences) can be loaded into memory registers by pressing CORR (or DCORR) on the keyboard (Fig 5).
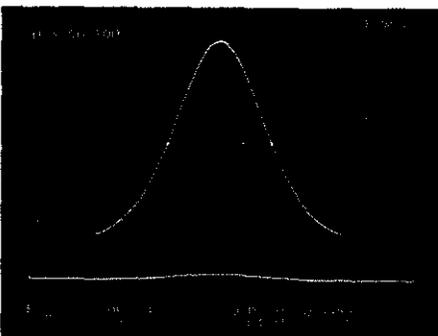

Figure 2 SCAMP CRT display. P and Q cursor coordinates on bottom of screen show position and intensity of data points. Up to four traces can be displayed, expanded, and massaged at one time. Here the cursors locate and define a peak's full width at half maximum (56.2 nm) as displayed in the Q cursor's H register.

Locating peaks and valleys is a pushbutton operation (PMAX, PMIN, Fig 3). So is sending the cursors to a particular horizontal (HSETP) or vertical (VLEVP) position. In this way you can quickly calculate the FWHM of a peak by pressing PMAX, QMAX, reading the intensity, loading half that value into the VLEVP and VLEVQ registers, then pressing DCOOR to display the difference between the cursor coordinates (Fig 2). There's also a peak-to-peak command (PK-PK) that locates the highest and lowest points between the cursors, positions the cursors at each one, and tabulates the difference in their heights.

SCAMP's nimble display formats have the unique power to present the intensities, or amplitudes, of a trace stored in one portion of the memory, as a function of those intensities stored in another, even if both traces are nonlinear. (In waveform analysis the result is a Lissajous figure, or a plot of Y_1 vs Y_2.) This was done in Fig 1 to plot differential temperature as a function of chamber temperature, but it is easily generalized to convert a spectrum generated as a function of wavelength to one displayed as a function of wavenumber, or energy, thus correlating the peaks with their corresponding energy bands to calculate quantum efficiencies and the like. Also,
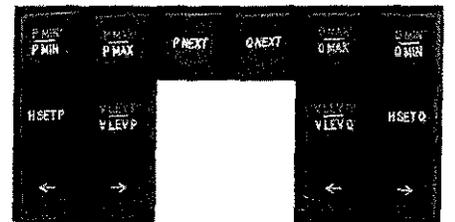

Figure 3 Cursor controls on SCAMP keyboard help isolate and quantify data parameters.
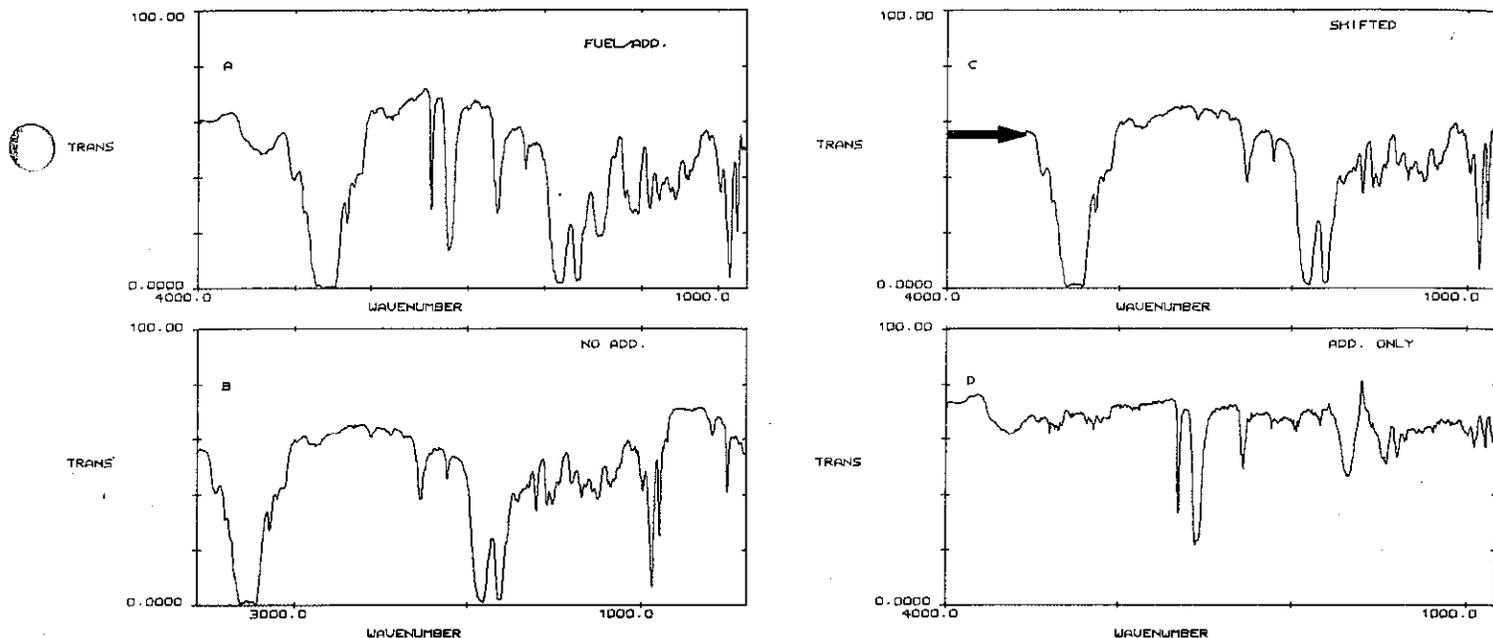
Figure 6 Some data systems might be stymied when faced with the task of producing the difference between a hydrocarbon fuel with (A) and without (B) a performance additive when the wavenumber regions of IR spectra do not match. Not SCAMP. A single keystroke command SHIFTs the additive-free spectrum the appropriate number of wavenumbers (C), making the subtraction possible and providing the spectrum of the additive alone (D).

calibration curves pop up in just about any form of analysis and, as we'll see, producing them is greatly simplified with this display proclivity, and the original data remains intact.

No system, however reliable, is immune to malfunctions so during warmup and initialization SCAMP makes a quick, though thorough, examination of its own health (Fig 4). A cyclical redundancy test (the sum of each hexadecimal word in the firmware) is performed on each chip, while the logic and timing of each circuit board are checked. The results are displayed on the CRT to pinpoint the source of a problem **before** you start taking data.

Figure 4 Every time you turn it on, SCAMP reports with a complete diagnostic display. Here the ROM/RAM software, DATA MEMORY, and DISPLAY boards are all OK, and the decimal sum of all 16 PROMS agrees with the check character. If it hadn't, a specific malfunction could be isolated by its hexadecimal code on the bottom of the display.

Fingertip Massage

If you assembled a panel of history's keenest mathematicians, each of them would probably choose to have a different pet function within easy reach. Newton and Leibniz would undoubtedly opt for integrals, both definite (INTPQ) and indefinite (INTPX). And Fourier would sneak his transform in somewhere (FT, IFT or Inverse). Still, others of a more analytical bent would rally for peak areas (PK-AR) and derivatives (D/DX) so changes in data could be located and quantified. There'd also be a powerful lobby for root-mean-square calculations (RMS), n-point averaging (NPAVG), and a statistical package to perform a linear regression analysis of data (STAT) complete with line parameters and standard deviations, through which data can be fitted to a theoretical model.
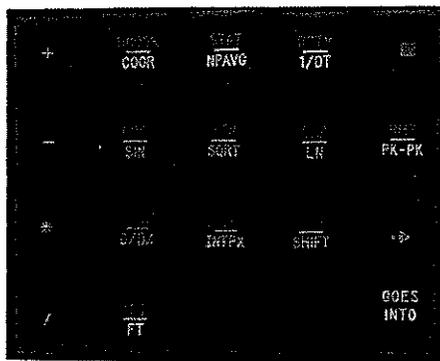

Figure 5 SCAMP's keystroke data routines turn operations as complex as Fourier Analysis into fingertip operations. And they can all be linked together into custom-tailored routines that automate complete experiments from data input to data output.

Rather than try to moderate among such demands, we included all those operations in SCAMP's repertoire, as well as the transcendental functions SIN, COS, ATN, SQRT, EXP, and LN which, aside from their normal uses, are especially valuable for converting data representations to those that are accessible to the statistical function. Nor did we neglect the arithmetic functions of addition, subtraction, multiplication, and division which can operate with equal effectiveness on all portions of the memory as well as any of 24 floating-point data registers (precision of 1 part in 16 million) and one integer register (I). As a bonus, any mathematical manipulation automatically adjusts the data to preserve maximum precision, thus eliminating the nuisance of constant rescaling.

The simplest of these operations, spectral subtraction, applies to Fig 6A which is the Infrared spectrum of a suspicious hydrocarbon fuel, containing a performance additive, that might have been found during the course of an arson investigation. B is an unimproved fuel. Subtracting B from A should yield the IR spectrum of the additive alone, which could then help tag the source of the accelerant. However, notice that the wavenumber regions of the two spectra do not match. Undaunted, SCAMP shifts spectrum B by the appropriate 400 wavenumbers (C) then calculates and plots the telltale difference spectrum in D. In a similar way, background or solvent blanks can be blocked out to leave only the data of interest.
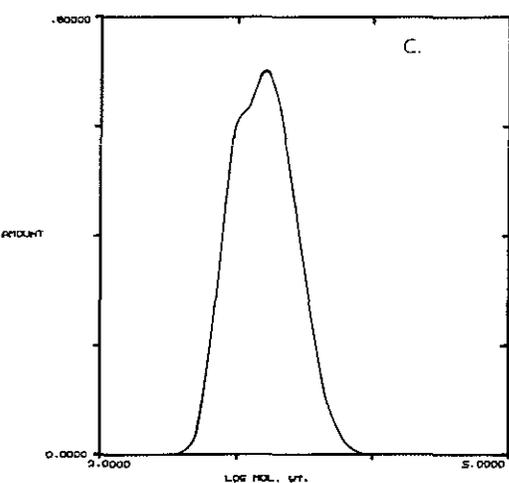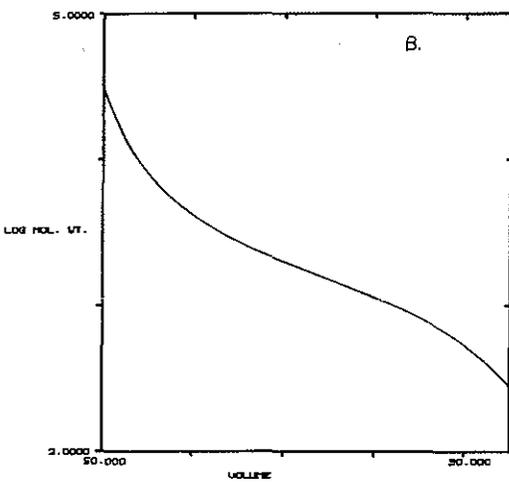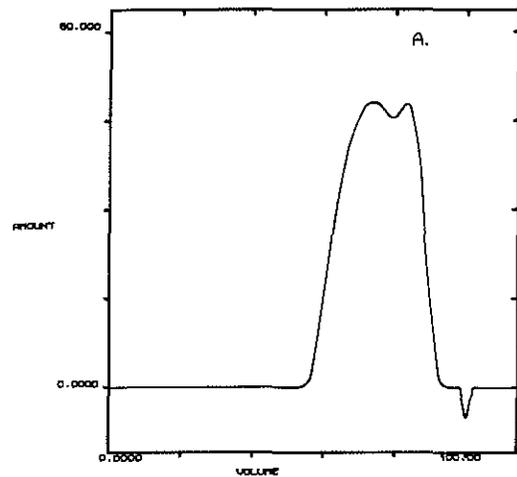
A.

B.

C.

Figure 7 GPC run of polyisobutylene. Normal or raw data (A) can mask the subtle changes that characterize or fingerprint a sample. However, displaying this data versus the calibration curve (B) results in a differential representation that even a novice has no trouble interpreting.

FIG 8

EU(BIPYRIDYL OXIDE)4 (CLO4)3 DECAY TRACED ON FLUOROLOG WITH PULSED-LAMP PHOS-PHORIMETER. LN OF DATA HAS SLOPE -1.1281. THE RECIPRO-CAL YIELDS THE LIFETIME 0.849 MSEC.

A. EU DECAY

B. LN OF DECAY
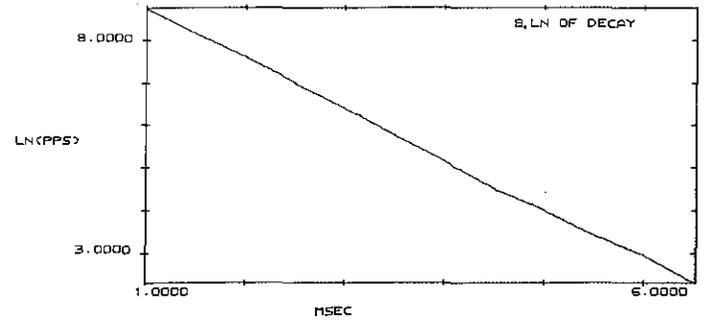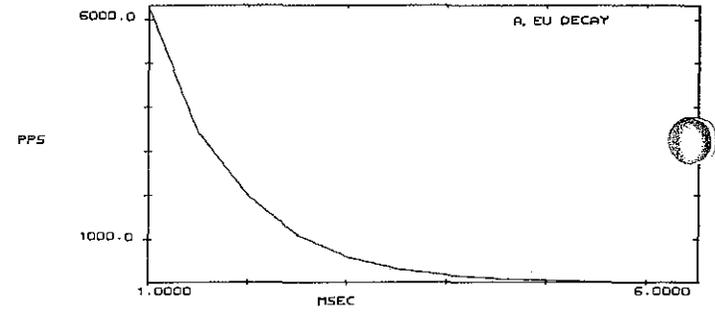
Gel Permeation Chromatography (GPC) (sorting sample components by their molecular weights) is a handy technique for quality control which virtually cries out for a data system to relieve it of tedious calculations. Number- and weight-average molecular weights are crucial to characterize polymers and otherwise must be carried out by manual digitization of chromatograms. Fig 7A [3], shows a GPC of a commercial sample of polyisobutylene (a principal component of STP — the racer's edge kind) that was taken as a function of sample volume (the small dimple at far right is air-water injected with the sample that sometimes serves as a calibration point). In this form, even a practiced eye can overlook the subtle variations that distinguish one sample from another, so the wary GPCer converts the data to a differential weight distribution with a nonlinear calibration curve like the one in 7B. Displaying A versus B yields the sought-after molecular weight distribution. The operator can now confidently go on to do the integrating necessary to calculate the average molecular weights.

Logarithms make lifetime and decay calculations a simple process of inspection. Phosphorescence intensity (I), for example, usually obeys an exponential law, after excitation is terminated, as it degenerates from its initial intensity (I_0).

$$I = I_0 e^{-t/\tau}$$

Here τ is the lifetime of the excited state, while t is the delay between excitation and sampling.

Taking the natural log yields

$$\ln I = \ln I_0 - t/\tau$$

a straight line with slope — $-1/\tau$

In Fig 8A we see a chart of such a decay from [Eu(bipyO$_2$)$_4$] (C10$_4$)$_3$ taken on the SPEX FLUOROLOG spectrofluorometer with our pulsed-lamp phosphorimeter [4]. B is the log. From the slope we easily find a lifetime of 0.849 msec.

Instead of manually calculating the slope, we might just as well have found it automatically by activating SCAMP's STAT function. It performs a linear regression analysis on the data isolated between the cursors, effectively fitting the best straight line that can be drawn through all the data points. STAT defines all the parameters listed in Table 1 and Fig 9.

What all this information can mean is demonstrated by following the evolution of the Atomic Absorption (AA) data shown in Fig 10. A is a typical run that might be generated when a known concentration of lead is determined. Ten readings were taken at the same concentration to gauge reproducibility. Combining the results from six such runs with six different concentration standards produces B, or AA response versus run number. In C, the concentration of each standard is plotted against its particular run number. By displaying B as a function of C, a calibration curve (AA response versus concentration) for this particular instrument is generated, though the curve is somewhat coarsely defined. However, by placing the cursors at opposite ends of the curve and pressing STAT, we obtain all the parameters SCAMP needs to generate the final working curve in E from which any subsequent AA run can easily establish the lead concentration in an unknown sample, as well as the relative error in each determination.

SCAMP's STAT function is equally effective at generating a straight line identical

Table 1 Curve parameters calculated by the STAT function.

$$\text{Mean Value of X (or Y)} = (1/N)\sum_{i=1}^{N} x_i$$

(N = # of points between cursors)

$$\text{Standard Deviation in X (or Y)} \quad S_x = \left\{ \left(\Sigma x^2 - (\Sigma x)^2/N \right)/(N-1) \right\}^{\frac{1}{2}}$$

$$\text{Slope of Fitted Line} = \Delta Y/\Delta X = \left\{ N\Sigma xy - \Sigma x\Sigma y \right\}/\left\{ N\Sigma x^2 - (\Sigma x)^2 \right\}$$

$$\text{Intercept of line} = Y_i = \left\{ \Sigma y \Sigma x^2 - \Sigma x \Sigma xy \right\}/\left\{ N\Sigma x^2 - (\Sigma x)^2 \right\}$$

$$\text{Coefficient of Determination} = \left(N\Sigma xy - \Sigma x\Sigma y \right)/N(N-1)S_x S_y$$
(Goodness of Fit)

to any sloping background that may be present in a spectrum. Unwanted contributions from the offending component may then be subtracted away.

Of course, all curves are not so cooperative as to follow a straight line, but many can be reduced to this form with the transcendental functions as demonstrated by the europium phosphorescence decay (Fig 8). And SCAMP's STAT function is hard to beat when calculating signal to noise, or finding half-wave potentials, or plotting activation energies, or...

Peak Performance

In any form of analysis, the information collects in those portions of the trace where changes are involved. Often they take the form of peaks, though they may also appear as rises in diffusion current, weight changes, or plateaus. In Thermogravimetric Analysis (TGA) plateaus can indicate temperature ranges of chemical stability, inflections the formation of intermediate compounds or changes of state. On the other hand, Mass Spec or EPR are primarily concerned with peak location. Even in Clinical Neurophysiology, a spike in an electroencephalogram can signal a major disturbance in the human brain. Depending on your interests, peak areas, integrals, derivatives — all have their individual stories to tell.

We've already shown how cursors can be positioned at maxima or minima, but a given curve may contain a host of bands all competing for attention like nestlings stretching toward the worm in their mother's mouth. Here peak to peak (PK-PK) is handy to locate the absolute maximum and minimum intensities between
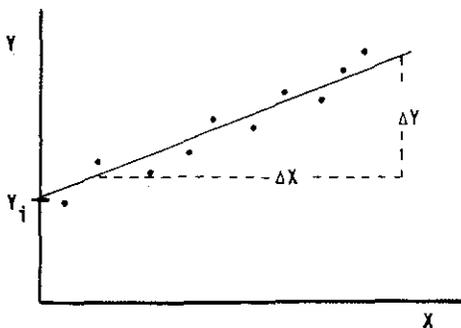

Figure 9 This sketch shows how SCAMP fits a straight line to scattered data with STAT.
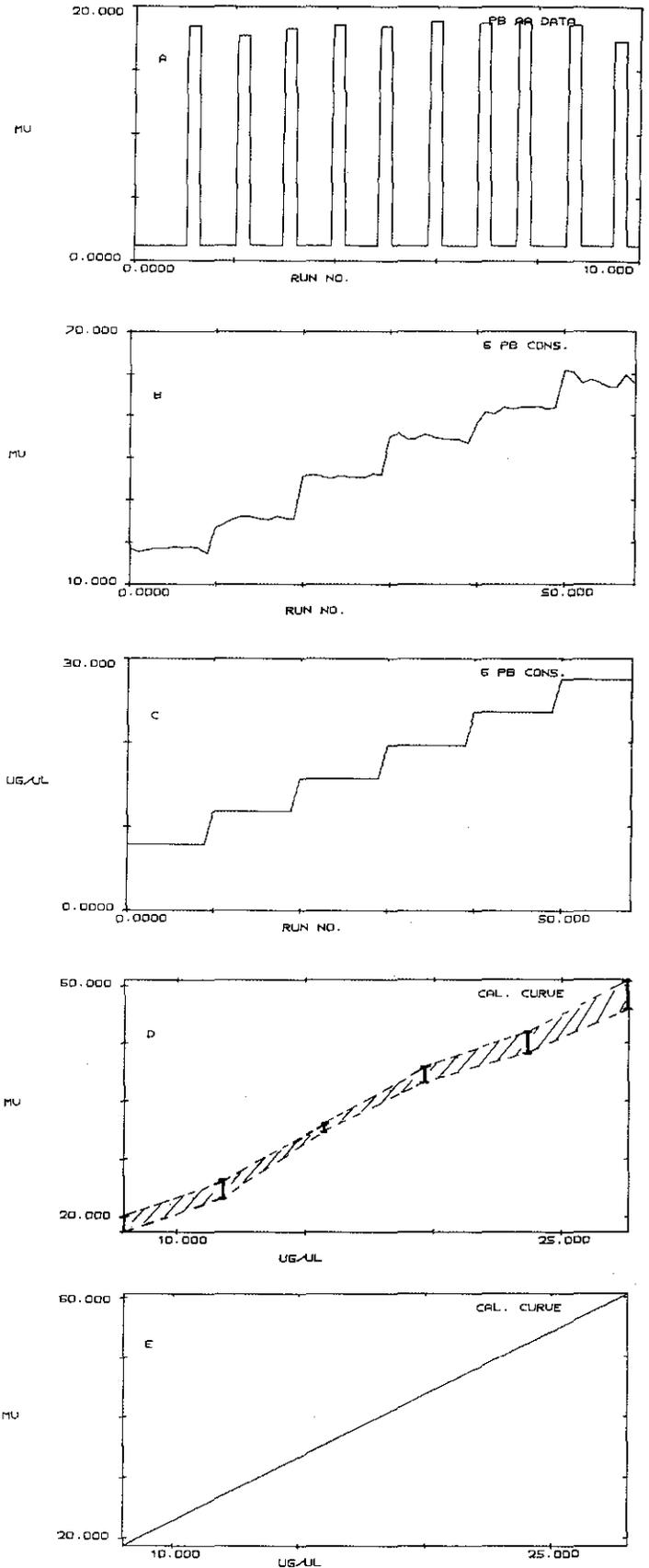

Figure 10 SCAMP calibrates an AA unit. Each known concentration of lead is sampled over a succession of 10 runs (A), then all such runs are plotted together in B. In C, the concentrations themselves have been plotted against run number. Displaying B vs C yields a calibration curve (the region we've shaded in plot D). With the STAT function, SCAMP then goes on to calculate the final working curve shown in E on which AA signals can be turned into concentrations simply by positioning the cursors.
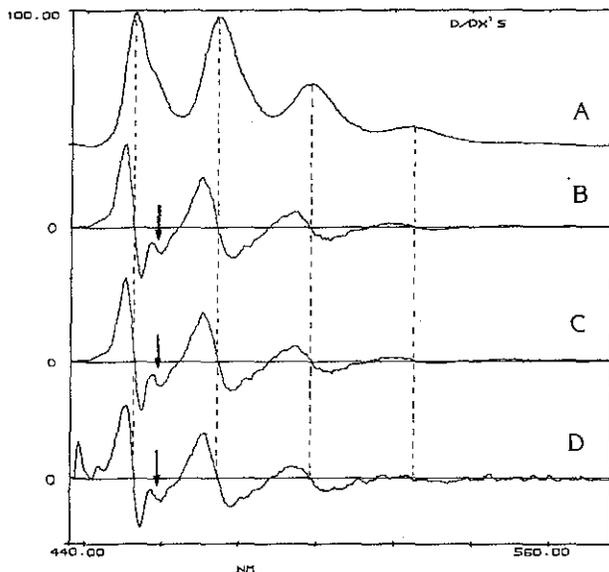
Figure 11 SCAMP differentiates a spectrum of anthracene to locate the peaks. B is the derivative taken with a keystroke command (D/DX), C a Savitsky-Golay 7-point derivative, D a Fourier transform derivative. Note that peaks occur where the derivative changes from positive to negative, valleys vice versa. Derivative spectroscopy sifts peaks out of broad backgrounds and overlapping bands. Note that the subtle shoulder in the lowest wavelength band is clearly positioned in all the derivative spectra.
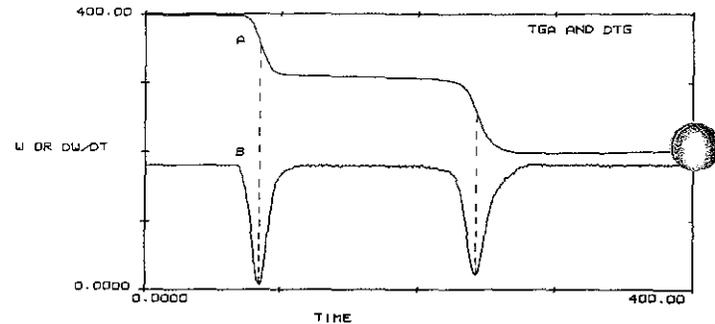

Figure 12 A DTG (Differential Thermogravimetric Analysis) curve is essentially equivalent to the derivative of a TGA (Thermogravimetric Analysis) curve.
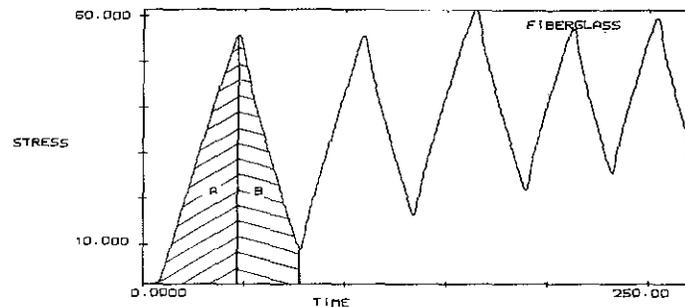

Figure 13 Here SCAMP converges on Sress/Strain Analysis when a strip of fiberglass is subjected to a cycling strain. The definite integral command calculates the areas A and B (the portions we've shaded), which are proportional to the energy absorbed, then liberated, by the sample. The difference (Q = A-B) is how much energy has been lost to the sample and tells a materials scientist how well the substance performs under load.

the cursors, while loading the difference in these two intensities into one of the registers. Thus, not only is the peak intensity available, but so is any baseline offset (the minimum) that might now be subtracted away. Another method particularly suited to sorting out overlapping bands or separating them from interferents, is differentiation. With SCAMP, applying D/DX to any curve yields the first derivative (Fig 11B). Note that both peaks and valleys are located at points where the differential intensity (I') equals zero, peaks crossing from positive to negative, valleys vice versa. This observation alone is equivalent to taking the 2nd derivative (applying D/DX again), noting that $I'' < 0$ for a maximum, $I'' > 0$ for a minimum, and since 2nd derivatives usually have extrema to either side of bands, they take the guesswork out of concentration measurements by defining the true limits of the bands [5]. Second derivatives have also been applied to detect the spike and wave in an EEG that indicates a patient has epilepsy [6]. Also note that the derivative of a TGA curve is equivalent to a DTG (Differential Thermogravimetric Analysis) curve (Fig 12), the DTG peaks, whose areas are proportional to the weight change of the sample, occurring at the center of the TGA rises.

On SCAMP, derivatives can be taken instantly with a single keystroke command, or by Savitsky-Golay convolutions [7] (Fig 11C), or by Fourier analysis [8,9]. In simplest terms, a Fourier transformation sorts a waveform spectrum according to which frequencies and intensities are necessary to reproduce its shape. To work this magic, a spectrum is converted to a complex representation having both

imaginary and real parts. The derivative theory of Fourier transforms [10] states that if the imaginary portion of the transform is multiplied by a linear ramp function starting at the origin, the result is the transform of the first derivative of the original spectrum. If you find that hard to digest, the results in Fig 11D should make things more palatable. Note how the gentle shoulder in the first peak is clearly defined in all forms of the derivative.

Once peaks are located, we want to extract all the information secreted in each of them. To do this we have at our disposal PK-AR (peak area), indefinite integral (INTPX), and the definite integral (INTPQ). Peak areas (the areas under curves that do not include the portions beneath an imaginary line drawn between the cursors) are essential when evaluating a concentration relative to a standard (Fig 1). In NMR, the area under a band is proportional to the number of a particular nuclei species responsible for that resonance, while in EPR, peak height is insignificant, but peak area reveals how many unpaired electrons are active in the sample. The list is endless. For each peak there is an area, for each area an application.

The definite integral (INTPQ), on the other hand, includes everything under the curve as shown in Fig 13 where a stress curve has been employed to evaluate the energy-absorbing character of a fiberglass sheet when it is subjected

to a cycling strain. (In this case, displaying stress as a function of time is most graphic, and just as easily handled by SCAMP.) The difference between the energy absorbed under strain (A) and that liberated (B) when the strain is eased (Q = A − B) determines the resilience and whether the material will best serve as a long-driving golf ball (small Q), or as a life-saving bumper to absorb the impact of a crash (large Q).

As we've seen above, the derivative in any of its operational forms, can enhance the resolution of spectra. On the other hand smoothing (which is essentially the 0th derivative) while improving the S/N and providing ego-boosting cosmetics, has quite the opposite effect: resolution is degraded to various degrees. Since no data reduction technique can be expected to extract more information from the data than was present in the original (but rather highlights features that may otherwise go unnoticed), there is always the question of trade off — S/N or resolution? Only the researcher can decide.

When it comes to smoothing, SCAMP again offers a choice of three types. By far the simplest and fastest smoothing is done by NPAVG, which is an unweighted average of 3 to 15 points. A tad more complicated, a Savitsky-Golay routine can be assembled by linking keystrokes as demonstrated in the following section. Finally, digital filtering with Fourier transforms is perhaps the most elegant
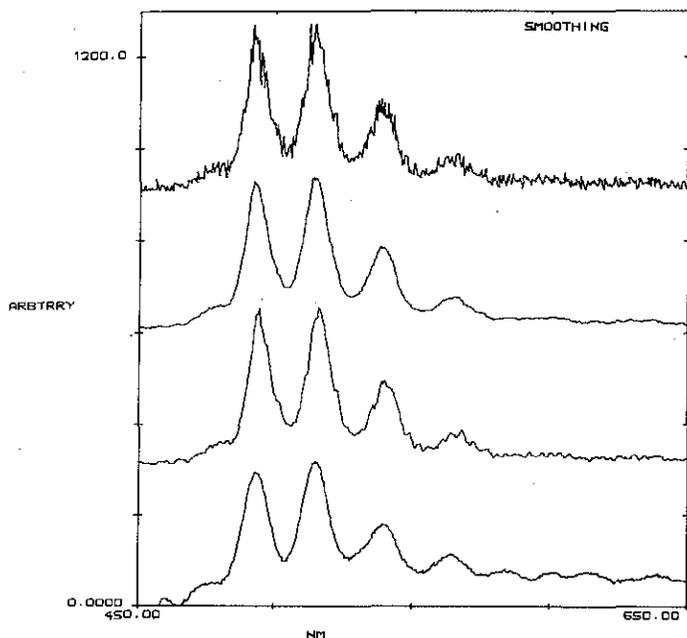
Figure 14 Three variations on smoothing with SCAMP. From the top: raw data, 7-pt NPAVG, 7-pt Savitsky-Golay, Fourier transform.
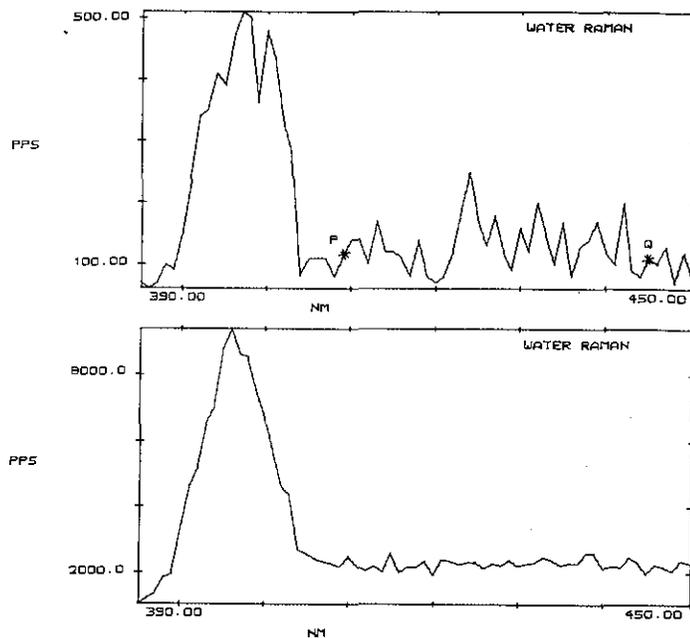

Figure 15 The top spectrum is a single scan with S/N of about 10. On the bottom SCAMP automatically rescanned the region, signal averaging until the S/N exceeded the operator's selection of 50. Only 18, rather than the expected 25, were enough.

smoothing technique, though its most profitable application takes a studied eye. Briefly, all components of the Fourier transform that are responsible for noise or distortion are blocked out with a window function before the inverse transform is applied. High-frequency components are usually manifestations of random noise or grass, while very low-frequency contributions could be the result of a baseline roll. Here the frequency we refer to is that relative to the width of the full data display.

A comparison of the three techniques is shown in Fig 14.

Keystroke Chains

Often the process of data reduction involves a number of distinct steps. You may wish to smooth the data before locating peaks, tabulating their positions, halfwidths, and areas. If the results are conclusive, you'll want to store them on a peripheral device before going on to take more data. Even though each operation in the sequence takes only a few keystrokes, before you're done finessing the information, you may have pushed ten, or even a hundred buttons if the refining process is particularly complex. Besides being tedious, repeating the sequence manually only invites mistakes. Fortunately, SCAMP's brain has two hemispheres: one to remember data, the other to learn a sequence of as many as 255 keystrokes which can be executed at the operator's convenience (with a disk option, the number of keystrokes is virtually unlimited). And because SCAMP's native tongue is the keystroke, there's no need to learn still another foreign language complete with

grammar and dialects. A quick example will show you what this can mean.

In Fig 15A we've run a Raman spectrum of water on the FLUOROLOG Spectrofluorometer with very tight slits. As might be expected, the scattering intensity is so feeble the signal has to compete against a gaggle of noise. You could, by hand, position the cursors to find the peak height, then move on to the noise at right, estimate its value relative to the peak to get the signal-to-noise ratio, and with that information decide how many scans it would take to drive the S/N within acceptable bounds. Finally, you tell SCAMP to run that many scans. When you're done, if everything went according to plan, you might have the spectrum you were looking for. And when you wanted to do the same to another spectrum, you'd have to go through the whole routine again.

OR, you could have SCAMP do it all.

Simply key the sequence of commands shown in Fig 16 into memory, position the cursors in a flat region of background to define the noise, and load in the desired S/N value. After that, running clean spectra is only a question of pushing SCAMP's RUN button. That's all there is to it — no subroutine matching, no indirect addressing, no bit shifting. It's as simple as operating a hand-held calculator.

Stringing keystrokes together in this way gives you the power to automate your work from input to output. In the AA example of Fig 10, for instance, SCAMP could be told to read the intensity from a sample, set the cursor to the corresponding level (VLEVP) and print out the matching concentration. And you

```
001    1.0000 ==> I
002    Q1 ==> Q2          Save the first scan
003    COOR               Then find out where
004    H - R3 ==> H        operator has positioned
005    H' - R3 ==> H'      cursors to define S/N
006    H / R5 ==> B
007    H' / R5 ==> C
008    B + 1024.0 ==> B
009    C + 1024.0 ==> C
010    SCAN               Get another scan
011    INCI               Keep count
012    Q2 + Q1 ==> Q2      Add new scan to old
013    B ==> HSETP
014    C ==> HSETQ         Return cursors to S/N region
015    HSETP
016    HSETQ
017    STAT Q2 VS T/F      Find standard deviation
018    1024.0 ==> HSETP    stored in D'
019    HSETP
020    PK-PK ==> D         Find peak intensity
021    D / D' ==> D        and calculate S/N
022    D IF > A
023    GOTO 26.            Good enough?
024    END                Then leave
025    GOTO 10.           Or scan again
026    PAUS
```

Figure 16 SCAMP lets you select your own S/N. Once you load the desired value (50 in this case) into the A register and position the cursors (Fig 15) you only have to press RUN and walk away. When you return, you'll find SCAMP waiting with a spectrum tailored to order.

The unannotated program above left is an example of SCAMP's serial printer output.

wouldn't have to be there looking over SCAMP's shoulder during the determination. We've assembled routines for running Raman spectra, then calculating the depolarization ratios of the lines, and all the operator had to do was press the RUN key and rotate the polarizer between runs — and even that could have been automated had we desired. SCAMP is just at home performing radiometric corrections, group scanning, or identifying peaks. Once unleashed, SCAMP buzzes on contentedly, taking data, extracting the information, deciding when it is good enough to meet your specifications, then presenting you with the finished product.

Of course, as soon as word of SCAMP's keystroke-linking memory spread, there were those who were ready to challenge the limits of its capability with increasingly more powerful combinations. One such application is curve resolving.

Overlapping peaks in a DSC (Differential Scanning Calorimetry) must be separated if one is to find the true shape and area of a sample transition. In X-ray and Fluorescence spectroscopy the precise number and locations of peaks testify to the electronic transitions and energy levels that hold the chemical world together.

At SPEX we've approached the problem of overlapping peaks with a deconvolution routine that rivals in complexity those designed to run on megabuck, megacomputers. Yet, again, the routine remains relatively simple thanks to keystroke linking [11].

After the operator determines peak shape and locates the peaks (with derivatives, PMAX, etc.), all that remains is a rough guess at the half-widths and peak intensities. SCAMP then goes on to assemble the specified number of peaks, adjusting them to fit the data and reiterating until a selected convergence criterion (the difference between the areas of the raw and deconvoluted spectra) is satisfied.

Consider the resonance spectrum in Fig 17 which displays the original scan of Ni complexed to 4(2-pyridylazo) resorcinol (PAR) and the curve generated by the deconvolution routine from peaks with the 30% Gaussian, 70% Lorentzian character typical of Raman spectra. The two traces are within 0.5% of one another. Below you see the five peaks that were actually resolved. Final peak positions, half-widths, and heights are also listed by the program.

Graphics and Disks

In the final analysis, the output tells the whole story. Except where necessary, all the data you've seen here, complete with comments, axes labelling, and titles, was routed through SCAMP's X-Y recorder. We call them report-ready graphs, for they need no additional arguments. They stand alone, speaking for themselves.

For mass storage, there's a floppy disk in which 99 Programs, 99 data quadrants (over 10^5 data points) and 99 full sets of registers can be stored, then called up whenever they are needed.
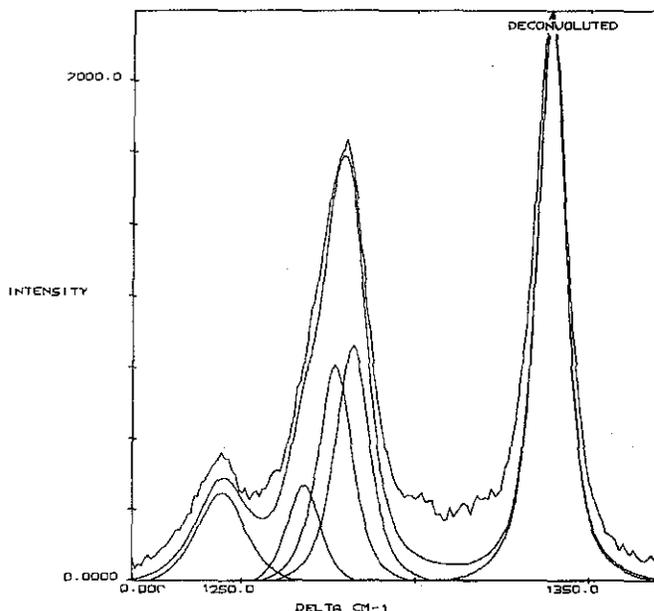

Figure 17 Raman spectrum of Ni complexed to PAR which SCAMP has resolved into five bands at 1244, 1268, 1277, 1282 and 1339 cm^{-1}. The difference in area between the raw and deconvoluted data is less than 0.5%.

A serial printer option is also available. Or plug in your own TI Silent 700, to copy data tables, registers, or programs.

And all peripheral operations can be performed under program control. We also understand that every research group has its computer fancier whose first question always begins with "Yes, but can we interface it to what we already have?" Well, the full complement of SCAMP's data is available on an RS-232 serial link [12].

In addition to all this, data taking can be initiated, halted, and reinitiated remotely when needed, and a signal can be sent by SCAMP to operate a sample changer, rotate a polarizer, or what have you.

The Last Word

That's yours, for in the end it's up to you. If you want to capture all the data there is to capture and wring out all the information nestling in valleys or squatting on peaks, then SCAMP is for you. There are other data systems. Some work on TGA's some on IR's, others on GC's. Then there's SCAMP, that works on TGA's AND IR's AND GC's, and just about anything else. When SCAMP goes on line in your lab, you decide what kind of data you want, in what form, and how much. SCAMP's portable, plug-inable, interchangeable, shareable — and, most of all, affordable.

No one knows your data as well as you do. But SCAMP knows where your data's hiding.

We've assembled a full set of Tech Notes further detailing SCAMP's wide-ranging applications and there's probably one that satisfies your particular demands. If you'd like to see more, just give us a call.

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