Vol. XIX No. 3 September, 1974

The SPEX Speaker

INDUSTRIES, INC. • 3880 PARK AVENUE • METUCHEN, N. J., 08840 • ☎ (201)-549-7144

THE RAMACOMP®- A COMPUTERIZED RAMAN SYSTEM

John F. Moore

SPECTROSCOPISTS labor under a computerized disadvantage. In the hands of astronomers, biologists, and rheologists, computers have been programmed to generate spectacular maps of Venus, vivid models of DNA, and realistic flow fields of hypersonic collisions. All make the cover of Science. By contrast, hapless spectroscopists are forever laden with reams and reams of dull and unimaginative graphs and computer-processed numerical data, which only rarely find their way even into the back pages of their own articles.

But, publicity aside, the computer has given a welcome assist to spectroscopy which is, by its very nature, a prolific source of difficult-to-manage data. Whether the task is to uncover a weak line buried beneath ubiquitous noise, or to extract the profiles of two overlapping lines, or to match an unknown spectrum with one already catalogued in a voluminous library, spectroscopists are often inundated with many meters of chart paper. For complete interpretation, they may need to analyze all of these data on a point-by-point basis. More than likely, a computer can make the difference between a job worth undertaking and one where interest in the results wanes faster than the time needed to interpret the data.

Until now much spectroscopic computer processing has been inefficiently done off-line. The spectrometer's intensity-vs-wavelength output must be transferred to magnetic or punched paper tape and then fed into a separate computer for processing. While this sequence is fine for locating a spectrum in a library, it is hardly suitable for improving or otherwise processing original data. In sharp contrast, a far less time-consuming approach is to unitize the entire operation. Spex has. In one self-contained system, the Ramacomp, data can be processed in real time. Moreover, and perhaps most important, the computer is given a free hand in optimizing the information during the time it is being generated.

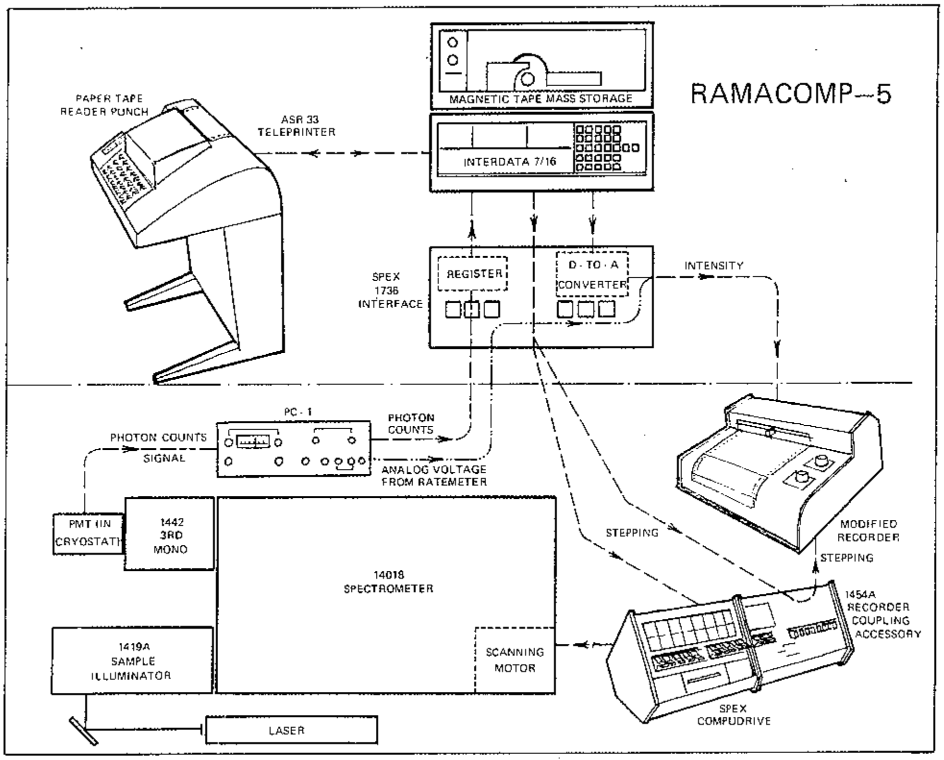


Fig. 1 The computerizing components of the Ramacomp are shown above the broken line. Below are units and accessories of the Ramalog.

Although what is emphasized in this paper are sub-routines related to Raman, Spex has participated in the manufacture of computerized systems spanning a variety of applications. Among these are systems for studying fluorescence, absorption, and emission; for characterizing the quantum efficiency response vs wavelength of photomultipliers for production control; for sorting of interference filters; and for conducting infrared luminescence research.

As diagramed in Fig. 1, the specially designed 1454A Recorder Control Accessory and 1736 16-Bit Computer Interface link the stripchart recorder to the Ramalog system, and the system to a 7/16 Interdata computer with 8K words of memory, a teleprinter, and a paper-tape reader and punch. This completes the standard Ramacomp package. Accessories presently include additional memory boards and a magnetic tape unit. With the latter, a large library of experimental spectra can be amassed, all rapidly accessible by the computer. Provisions have been incorporated to add a graphic display terminal, this device having already proved so valuable in other areas of science. It plots on a TV screen in real time, can also include coordinates and a listing of the material and conditions under which the data were taken, and can even dispense a hard copy of the graph which is "printer ready."

The particular computer was singled out for a variety of reasons. Well aware that much analytical equipment and many laboratories themselves were already equipped with or committed to minicomputers, our first impulse was to incorporate one of the more common types: DEC's PDP or Data General's Nova. Upon further investigation, we found that a comparatively new entry into the minicomputer field, Interdata Corporation (now a subsidiary of Perkin-Elmer) was offering more memory for the money, an assembly language and architecture resembling those of IBM, and a number of hardwired features which in other computers would entail additional software.

In choosing the Interdata 7/16 for the Ramacomp, however, we made sure not to lock the door against those researchers already committed to other minicomputers. The master key is the Spex 1736 Interface, designed not only as a component in our Ramacomp, but as a separate unit to go between our current spectrometers and any 16-bit computer. In fact, it may also be interfaced to an 8- or 12-bit computer through an 8-bit "hold" module. Requiring 4 command lines and providing up to 8 status lines, the 1736 Interface handles many functions. It processes intensity either in photon-counting or analog form. It can help the computer monitor the status of experimental functions and control signals for such operations as insertion of filters, polarization analyzers, and polarization rotators. The Interface also operates the pen lift, marker pen, and stepper motor of the stripchart recorder.

Incidently, the stripchart recorder has been retained in the Spex Ramacomp. Although every young computer specialist will authoritatively explain to his elders that plotting data on a stripchart recorder is a foolish reversion to an obsolete means of data presentation, yielding nothing beyond what the computer can reveal digitally, tradition still reigns. It may be that the human mind performs in analog fashion. Through the eye, it can examine the nuances, dips, and whirls of a spectrum and somehow arrive at interpretations more comfortably and rapidly than from listings of numbers.

And, despite the further admonition of our computer-sufficiency enthusiasts to the contrary, we have also made sure that all components in the Ramacomp can be operated manually as well as via computer. For the manual mode the PC-1 photon-counting unit is equipped with a ratemeter which feeds an analog signal directly to the recorder pen amplifier; the stepping motor in the recorder paper feed may be switched to the divider network in the Recorder Control Accessory to vary the chart scale presentation; and the scanning motor in the spectrometer is controlled by its own Compudrive.

Fig. 2 is a copy of the parameter table through which the computer is told how to run the system. The first six items are passive, serving mainly as a check list and permanent record. The remaining items are interactive, directing the computer to execute what the operator legislates. No. 7, incidentally, is a safety flag, preventing damage to the photomultiplier. Should the computer inadvertently be directed to scan through the laser line at 19435 cm⁻¹, ever-alert, it would cause the spectrometer to pause and issue a warning. "CAUTION LASER LINE." The operator can, if he then wishes, take the responsibility for scanning through the laser line by typing, "CO" for continue.

No. 8 is for calibration. When "CA" is typed the spectrometer will automatically scan to what it thinks is the calibration frequency, 19000 cm⁻¹. Note that this is a safe distance away from the laser line. If, in the interim, someone has twiddled with the knobs, the wavelength of the spectrometer can be readjusted manually.

No. 9 informs the computer that the instrument is calibrated in wavenumber and is fitted with gears such that each motor step equals 0.02 cm⁻¹. Other Spex instruments are linear in wavelength, and some have different gear ratios.

No. 10 offers three choices: No, Stokes, and anti-Stokes. With the latter two, scan commands are read in delta rather than absolute wavenumber.

Camouflaged by the title "RESOLUTION," No. 11 embodies one of the most powerful features of the software: the choice of either continuous scanning or taking of data at points with any desired spacing. Had the number 0.02 been substituted for 0.5, the computer would scan in normal manual fashion, burdening its memory with 50 intensity values per wavenumber. This is appropriate for spectra with the highest resolution, but otherwise is wasteful of memory capacity. In the "burst mode" (denoted by the choice of any larger number than 0.02), data are taken at larger intervals; the entry 0.5 causes data to be taken twice per wavenumber. Such data are, however, affected by the parameters given in 12-15. Together, the maximum time, the minimum time, and photon counts determine whether the spectrometer will be running at a constant rate, at a variable scanning rate such that constant-intensity values are fed to memory, or a combination of the two. Constant scanning rate is a simple case which offers little more than manual scanning; scanning is not optimized while the data are being generated. For the record, it is achieved by setting No. 12 and 13 equal to one another.

PARAMETER TABLE

```
:-LIST
1  OPERATOR:-              A.W.PROTIN
2  DATE:-                  30 SEPT 74
3  SAMPLE:-                415
4  REMARKS:-               TWO COMPONENT MIXTURE
5  LASER:-                 SP165
6    POWER:-               300 MW
7    LINE:-                19435CM
8  CALIB:-                 19000CM
9. STEP SIZE:-             50CM STEPS/UNIT
10  RAMAN:-                ST
11  RESOLUTION:-           0.5 UNITS/DATA POINT
12  MAX TIME:-             2.5 SECS
13  MIN TIME:-             0 SECS
14  PHOTON COUNTS:-        1000 COUNTS
15  MIN RATE:-             400 COUNTS/SEC
16  NO. SCANS:-            1 SCANS
17  SLITS:-                30/60/30 MICRONS
18  POLARIZER:-            NO CODE
19  ANALYZER:-             NO CODE
20  SCALE:-                10 UNITS/CM
21  MARKER:-               20 DATA POINTS/MARK



:-PLOT 1500CM,2000,A

SET PARAMETERS:-
22  100%:-                 5E4 COUNTS/SEC
23    0%:-                 400 COUNTS/SEC
:-
```

Fig. 2 Computer printout of the parameter table by which the computer is instructed how to direct the system.

If, on the other hand, parameters 12-15 are chosen as shown, scanning is accomplished in a fashion that optimizes the combination of signal-to-noise and scanning time. It is significant to note that No. 12 and 13 override No. 14. That is, if insufficient signal is received in the allotted time, the computer directs the spectrometer to move on to the next data point. It is often advisable to run a fast survey scan first as a guide to setting these parameters most effectively.

Let's take a hypothetical example to illustrate what happens in a typical Raman spectrum. Usually the region 1500-1800 cm⁻¹ is free of Raman lines. With the parameters in Fig. 2, the spectrometer moves 0.5 cm⁻¹ (25 steps) for a measurement. Here, another feature of the software should be mentioned. It has been constructed so that the computer looks at the register at intervals of 1/32 of a second; when it does, it transfers the count to its memory, and resets the register to zero. The first of these look intervals is used as a "quick look"; if the count is less than 1/32 of the minimum count rate set in Parameter 15, the computer concludes that the intensity is too low to be of interest, and immediately steps the scanning motor to the next data point. It can thus scan the 1500-1800 cm⁻¹ region in 20 seconds.

Now let's see what happens when a weak line appears at 1850 cm⁻¹. If the computer sees a value higher than 1/32 of the minimum count rate (in our example, 13 counts or more, giving a rate of 416 counts/sec or more) it keeps the spectrometer at that setting; every 1/32 second it rechecks and resets the register and adds its count to an accumulating total in the computer's own memory. It continues to do so until the count reaches the fixed value in Parameter 14, unless the maximum time in Parameter 12 expires first. In our example, if the rate is just over 400, it will take 2.5 seconds to reach 1000; since we allowed for this maximum, time will never run out first. As the spectrometer moves into regions of stronger signal, the register will fill up more in each look period. As long as it fills to 4095 or less (corresponding to rates below 131040 counts/sec) operation will be as just described above. With still higher count rates, more than 4095 counts will enter the register in 1/32 of a second; since it has 12 bits, it will "roll over," starting again to build its count up from zero. The software adds 4096 for every rollover signal that it receives before the end of a 1/32 second look period.

With stronger signals, obviously the time needed to reach 1000 counts will be shorter; scanning speed will increase at a rate proportional to signal level. Put another way, such signals will be measured not for a constant time but until a constant count is built up. Mathematically, this yields a constant signal-to-noise ratio. Of course, the constant count output is not meaningful of itself. The software divides this fixed count value by the varying time, giving a varying rate in counts/second which is proportional to intensity. Naturally, during all of this juggling, the computer is simultaneously controlling the chart-feed of the recorder.

With or without the constant signal-to noise mode, there is one beautiful advantage to stopping the scanning drive while collecting photon counts: freedom from time-constant error. Spectroscopists are used to a three-way trade-off, relating the spectral slit width and the scanning rate to the time constant. If RC is too small, noise will be excessive; but if too large, the time constant will not respond fully to the sudden swing of a sharp peak and its height will be recorded incorrectly. In the Ramacomp. the tradeoff is only between noise and dwell time at each data point, with separate independent selection of the number of data points per spectral slit width (10 are usually sufficient). But the height of a peak is always preserved; this is so because each data point is processed independently of all others.

The actual measurement of intensity is even more involved than that already outlined. Before describing this, let us recall the interrelated limitations inherent when analog signals are read in the normal fashion: one must trade off dynamic range and readout accuracy, with the result that both are usually sacrificed. The dynamic range of a typical meter or stripchart recorder is around 100:1. Since it is practical to read to an accuracy of around 1/2 division, the relative readout error is equally variable. At the lowest value of one unit, the error can be as poor as 50%; at the highest value, it is reduced to an acceptable 0.5%. At the same time, the measuring technique is confined to a narrow dynamic range which can be extended only by switching either automatically or manually.

The relative freedom with our software is evident. Here the full dynamic range of the photomultiplier and photon counting system – in excess of 1.5 million – can be exploited without switching and with an error never exceeding 0.025% in computation and 0.1% in output. Accomplishing this is straightforward with the Spex Interface.

First, the capacity of the register in the Interface, which has a dynamic range of only 4096 (12 bits), must somehow be raised 500 times to handle a photon counting rate of 1.5 million (21 bits). As mentioned above, whenever the register in the Interface reaches its 12-bit maximum it "rolls over," starting once again at zero. Simply by counting the number of rollover signals and adding 4096 times this figure to the number of counts remaining in the interface register, the computer is able to store the desired 1.5-million range of intensity values.

Since the computer handles 16-bit words, one might understandably question how it copes with numbers as large as 21 bits and – in computations – even larger. This is done by putting the numbers into a floating-point format. After the computer divides the number of counts by the time taken to reach that signal level, it translates this number into one with 12 bits of magnitude and 4 bits of exponent. Up to 134.2 million counts can thus be stored in memory. Although, as already indicated, the photon counting system remains linear to only 1.5 million, the added capacity permits summing intensity values in replicate scans for purposes of computer averaging, as well as in other computations where intermediate numbers become large.

This overall approach to measuring signal levels is especially significant in many Raman measurements. A common problem, for example, is to measure one substance at a trace level mixed in a solvent. Following customary practice in analytical chemistry, it is best to take the ratio of intensity of the unknown line to that of an internal standard line in the solvent. Thus, a weak line must be measured immediately before a strong one. Obviously, the greater the accuracy in measuring both, the greater will be the calculated precision of the actual concentration.

As important as the measurement of intensity is the control of the spectrometer's stepping motor by software. When the desired starting and terminating delta wavenumber range is entered as part of the "SCAN" command, the computer immediately drives the spectrometer to the starting value, either forward or backward, as indicated. Whenever it is stepped backward, an overshoot of 10 cm^{-1}, followed by forward motion to the starting wavenumber, eliminates backlash. All of this is done exceedingly rapidly through so-called ramping circuitry: for a stepping motor to reach reasonably high speed, it must be accelerated, the train of drive pulses being sent to it at a steadily increasing rate. It must also be ramped downward at the end of a high-speed run. Further, parameter No. 16 may be edited to up to 999 scans for signal averaging.

At this point, No. 17-19 are passive parameters. Although provisions are included in the Interface for controlling each of these functions, mechanisms are not yet available for carrying them out.

No. 20 is directed to the stepping motor of the recorder. In this case, the paper feed is adjusted so it moves along at a rate of 10 cm^{-1} per cm of paper. Should one wish to operate in the infrared-compatible mode, No. 20 is set to read "IR."

No. 21 furnishes the marker blips, here every 10 cm^{-1} (20 data points/mark x 0.5 cm/data point).

No. 22 and 23 set the intensity range of the recorder. The recorder pen will swing full scale when it receives 50000 counts/second (5E4) and will drop to zero at the general background level of 400 counts/second.

The most extensive software area embraces a set of subroutines involving computation. These extend from relatively straightforward ones handled automatically by the software to exceedingly complex ones, those that "massage" the data to produce enhancement and comparisons that have proved so time-saving and beneficial.

Automatic computations include:

1. The summed intensity of multiple scans is divided by the number of scans. Obviously, this accomplishes signal averaging. For the computer to sum intensities at a particular wavelength without loss of spectral resolution, not only is it necessary that the computer keep exact count of the channel being read but the spectrometer must not drift from one scan to the next. Under conditions of highest optical resolution (around 0.2 cm^{-1}), the spectrometer is taxed because points are

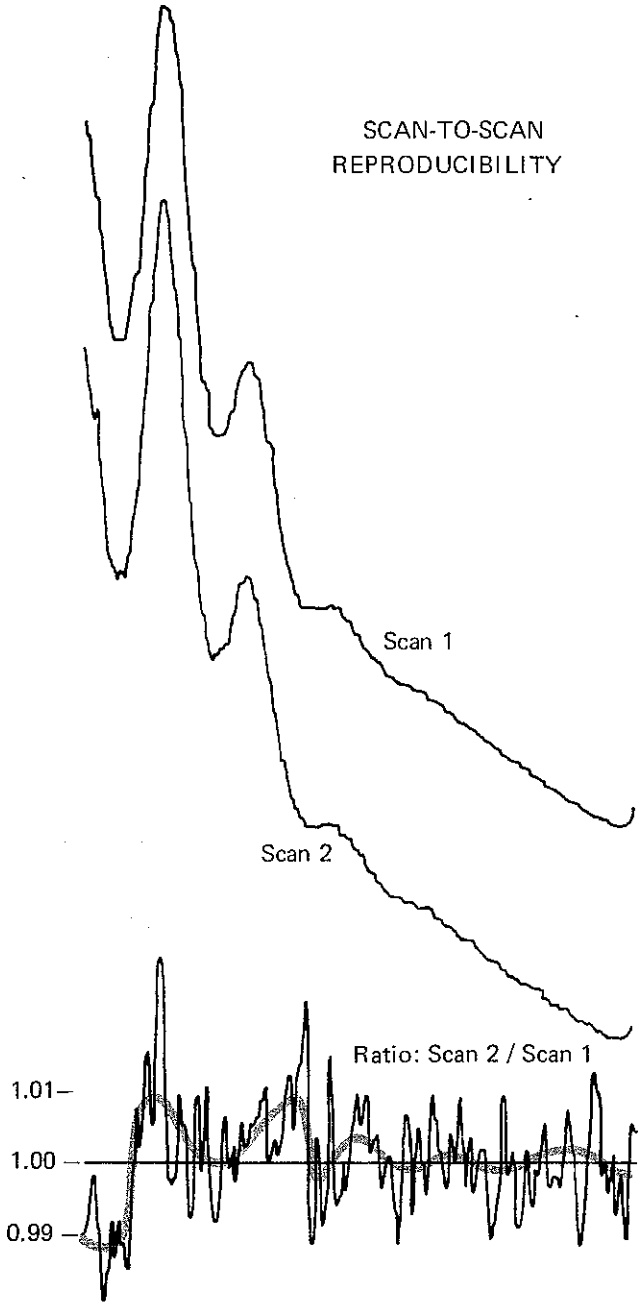


Fig. 3 Identical traces were taken and then ratioed to determine the total amount of drift in the scanning system. The fluctuations in ratio, less than 0.5%, indicate excellent system reproducibility.

read every 0.02 cm^{-1}. We have shown that short-term, scan-to-scan drift is less than a single motor step. Of course, strict control of the temperature of the spectrometer must be maintained to avoid long-term drift.

2. Interpolation of curves in memory is provided. To instruct the recorder pen to draw a smooth line between the measured spectral data points, the computer routinely estimates the in-between points on the chart.

3. Signal to the recorder is adjusted so its pen always remains on scale. Simply – though inadequately – explained, before the computer tells the recorder how to draw a curve from the digital information in its array, it searches for the most and least intense values. The least intense value (and thus the entire curve) is brought down toward zero by subtraction of a constant. The most intense value is then multiplied by a suitable constant so it falls in the upper half of the chart. To superimpose two related spectra for comparison, a "RETRACE" instruction and one to "FIX" the scale are also within the "PLOT" command. Of course, all this automation may be overriden at will.

4. The scan rate of the spectrometer can be controlled. In the simplest operating mode, the scan speed is stepped at a constant rate while the computer is instructed to take intensity measurements at fixed increments. In another, the "burst mode," the scan is made rapidly between measuring points where the spectrometer dwells. As discussed earlier, the dwell time can be set for a fixed time or until a pre-determined number of intensity counts is received.

But "data manipulation" is the real payoff. Interacting through the teleprinter with the computer, we can call for any of a number of powerful mathematical treatments which, individually or reinforcing one another, are exceedingly valuable. The simplest involves manipulating data stored in a particular array. Software can take logarithms, the absolute values of the first or second derivative, or it can integrate an area in a selected interval. Further, it can smooth a curve (squelching noise blips by the method of least squares) or

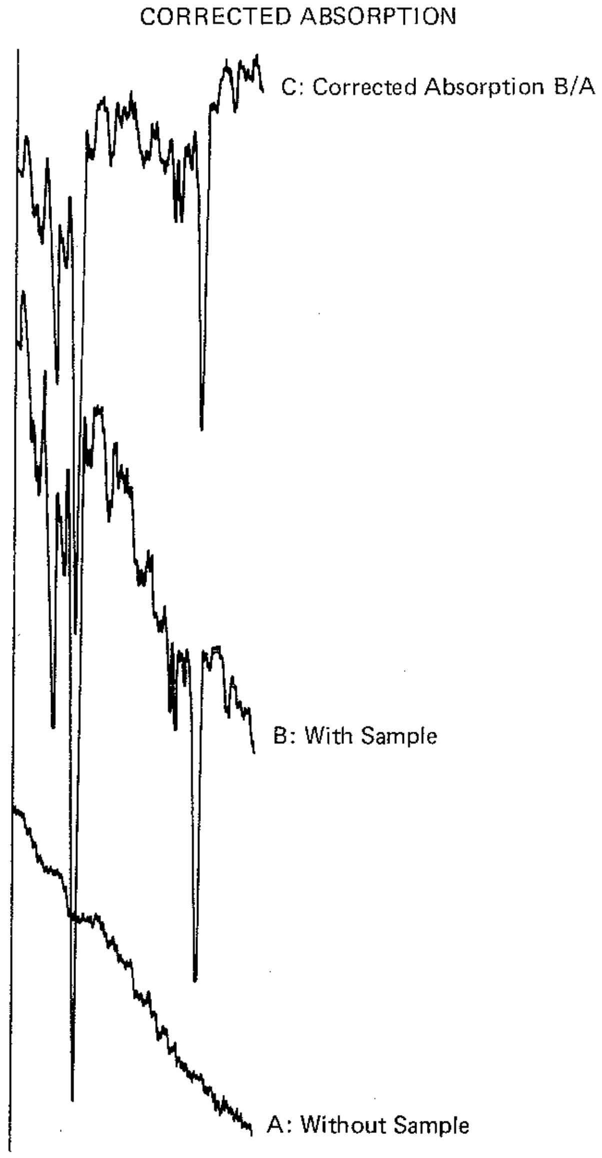


Fig. 4 A bonus feature of our software is its ability to take corrected absorption spectra. Tracing B is of a sample of benzene in its fused silica cell while tracing A is of the empty cell alone. Towards shorter frequencies, the overall intensity of the source as relayed by the PMT steadily drops. When the two are ratioed, as in tracing C, the true absorption spectrum of benzene emerges, corrected for variations in the source, the optics, and the detector.

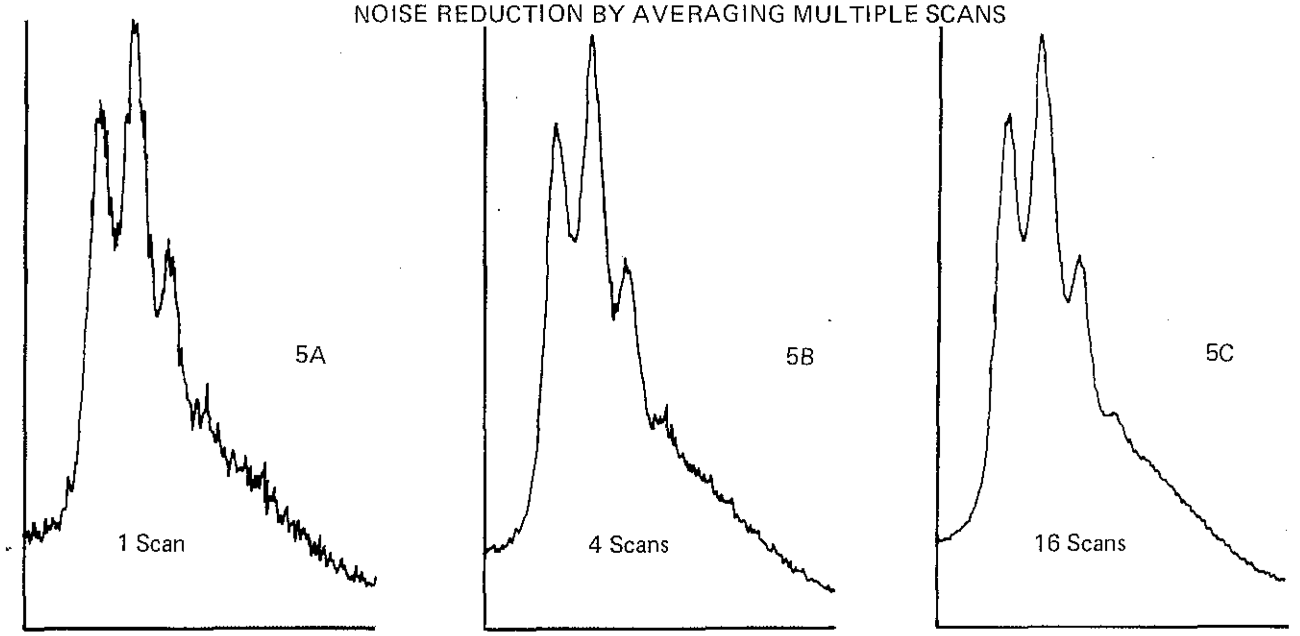

NOISE REDUCTION BY AVERAGING MULTIPLE SCANS

Fig. 5 Indicated in 5A is the noise suppression achievable by just a single treatment: multiple scanning. Here the 459 cm^{-1} line of CCl_4 was first scanned in 15 seconds; 5B and 5C present the average of 4 and 16 such scans, respectively. Incidentally, to stress the noise depicted in 5A, a number of monkey wrenches were thrown into the parameters: Slits were narrowed to 30 microns, dwell time was reduced to 0.05 seconds per point and the laser intensity was deliberately turned down. The overall signal-to-noise improvement evident in progressing from one scan to 16 scans is what statistics predict: about four-fold. At the same time, it is to be noted that resolution has not deteriorated, a tribute to the reproducibility of the scanning mechanism of the spectrometer.

print out the most intense peaks in order of their wavelength (or wavenumber) or intensity. With an instrument linear in wavenumber, scans linear in wavelength can be produced or vice versa. And, finally, many of these sub-routines can be combined and then displayed on the stripchart recorder tracing.

Fig. 3 & 4 illustrate ratioing of two spectra, often done to record depolarization ratios automatically. Here, other purposes were achieved.

Fig. 5 & 6 illustrate the combination of two statistical treatments to save a good deal of time in optimizing signal-to-noise. It is true that, statistically, the four-fold S/N improvement achieved is equivalent to a single scan taken at a rate 1/16 the speed of that in Fig. 5A. But slow scans are much more susceptible to instrument drift and certain other sources of noise. Furthermore, with multiple scanning, the spectroscopist can examine the entire spectrum periodically; he does not have to wait hours before shutting down a bad run.

But for scanning 1150-1450 cm^{-1}, which took 5 minutes each, the S/N improvement evidenced in 6C would have taken nearly 150 repetative scans and more than 7 hours. According to Savitsky and Golay, in an article on smoothing, (Anal. Chem. 36, 1627, 1964), "The use of combined smoothing and averaging can considerably reduce the instrument time required [to enhance signal-to-noise] throwing the burden on the computer, which operates in a wholly different time domain. A characteristic of both procedures is that the noise is reduced approximately as the square root of the number of points used."

NOISE REDUCTION BY COMBINING TWO TECHNIQUES

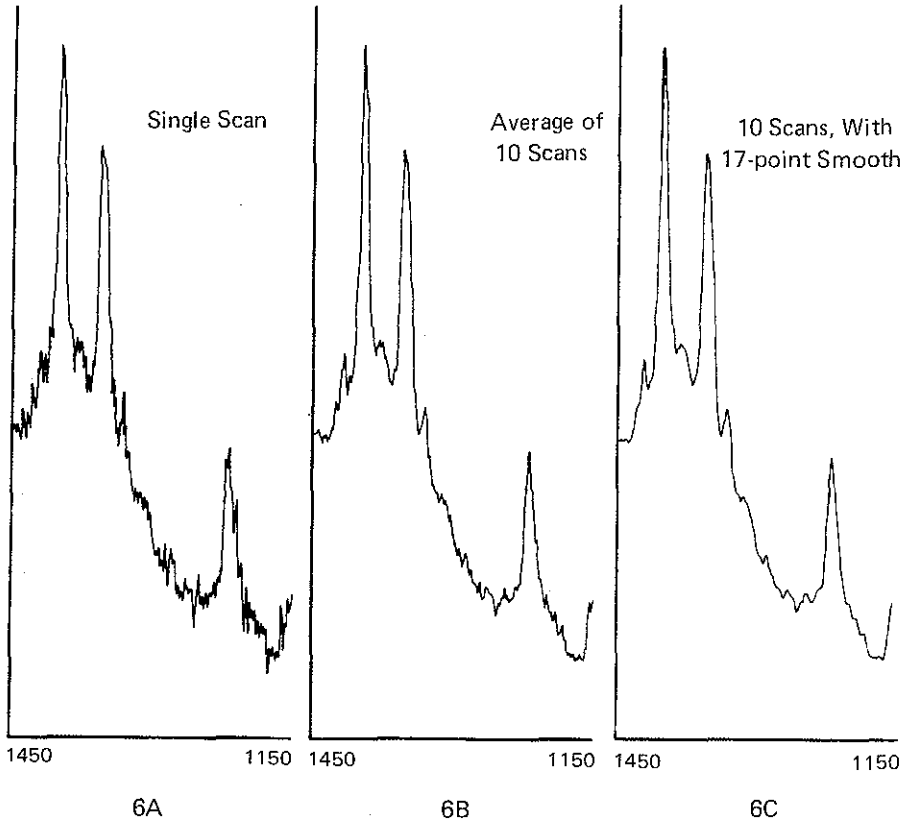


Fig. 6 The results of combining two statistical treatments of signal-to-noise ratio. One is signal averaging through multiple scans; the other is smoothing. Unlike the spectrum of the 459 cm^{-1} structure in Fig. 5A, here a single scan of the region 1150-1450 cm^{-1} was quite slow, taking about 5 minutes. Ten repetitive scans in 6B thus took almost one hour to achieve only a three-fold improvement in S/N. It took the computer an additional 10 seconds or so to mull over the data in 6B in a 17-point smoothing routine. The result, in 6C, is a further four-fold improvement in S/N.

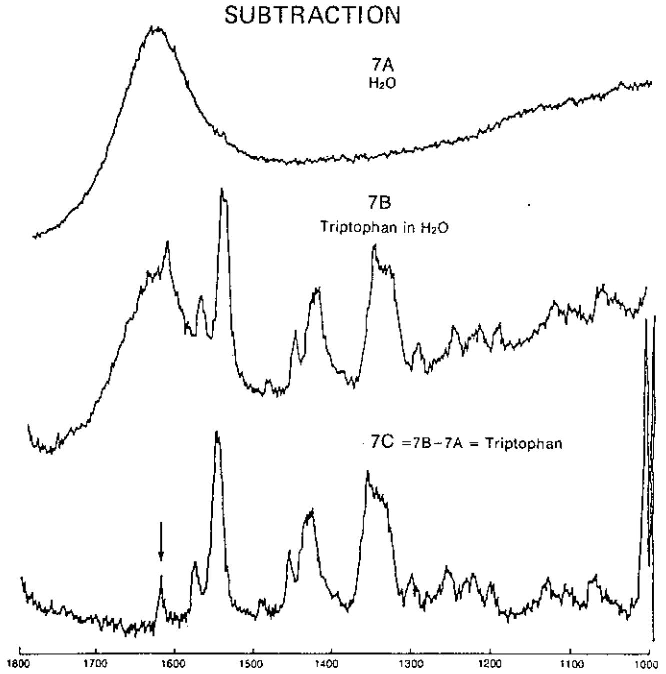


Fig. 7 Here a solvent effect is removed by subtraction of spectra. Because Triptophan dissolves to such a limited extent, the high concentration of water can give rise to severe interference by its spectrum. The 1610 cm^{-1} line might understandably be confused with noise in the spectrum of the mixture but in 7C it clearly becomes a "real" feature.

Although the results shown in Fig. 6 were obtained with a 17-point scan, the sub-routines available include options from 5 points to 17. The need for these is to prevent over-smoothing with subsequent loss of real spectral features. Statistically, the best smoothing is that with the most points, as long as there are no more smoothing points than there are data points in the half-power full-width of the narrowest line. As long as this condition is met, the true peak value and the shape of the peak remain essentially undistorted. Therefore, if scanning time has been reduced by taking, say, 10 data points per peak width, a 9-point smooth is most appropriate.

An example of separating the spectrum of a solvent from that of a sample is given in Fig. 7.

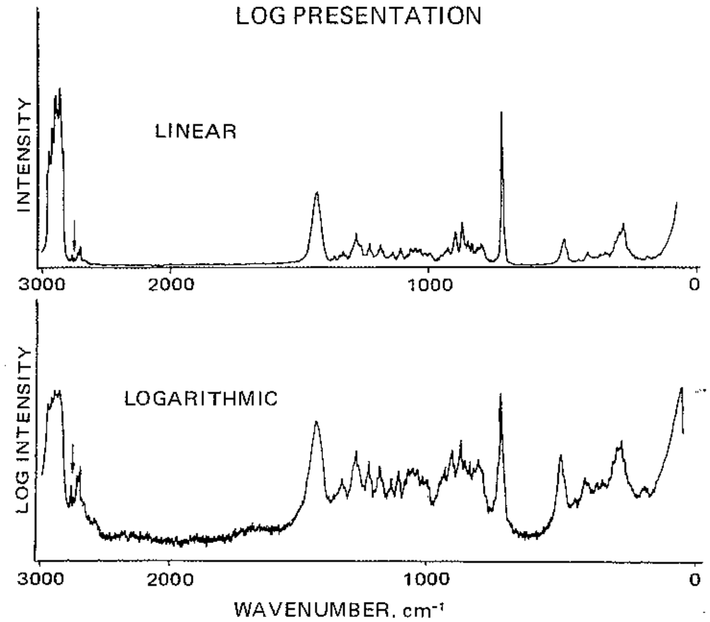
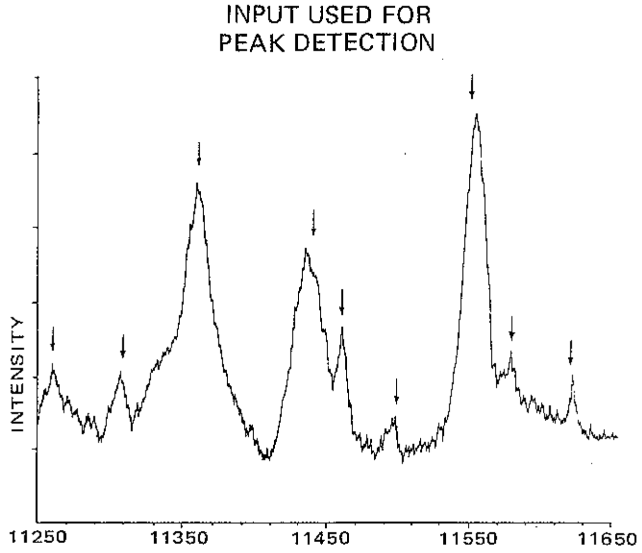


Fig. 8 A comparison, in IR format, of a linear with a logarithmic presentation of a pair of weak peaks near 2750 cm^{-1}. Material is a mixed hydrocarbon.



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:-RANGE %, 11650CM, 11250

    8655      AU    11550CM      5348      5348
    8832.856  AU    11360CM      4538      4538
    8741.807  AU    11440CM      3427      3427
    8726      AU    11460CM      2512      2510
    8636      AU    11580CM      2338      2338
    8830.985  AU    11260CM      2062      2262
    8841.935  AU    11310CM      1794      1794
    8695.987  AU    11580CM      1443      1443
    8625.939  AU    11620CM      1324      1324


    8625.833  AU    11620CM      1324      1324
    8635.568  AU    11580CM      2338      2338
    8658      AU    11550CM      5348      5348
    8695.641  AU    11580CM      1443      1443
    8726      AU    11460CM      2510      2510
    8741.243  AU    11440CM      3427      3427
    8832.867  AU    11360CM      4538      4538
    8841.723  AU    11310CM      1794      1794
    8880.934  AU    11260CM      2062      2062


    8830.984  AU·   11260CM      2062      2062
    8841.985  AU    11310CM      1794      1794
    8832.985  AU    11360CM      4538      4538
    8741.248  AU    11440CM      3427      3427
    8726.248  AU    11460CM      2510      2510
    8696.249  AU    11580CM      1443      1443
    8658.249  AU    11550CM      5348      5348
    8636.249  AU    11580CM      2338      2338
    8696.25   AU    11620CM      1324      1324
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Fig. 9 The three printouts are actually rearrangements of the same data: the first is in order of decreasing intensity, the second is in increasing wavelength, and the third in increasing wavenumber. Normally only the desired presentation appears.

Fig. 8 shows how a pair of weak peaks near 2750 cm^{-1} might easily be missed in a linear display but are clearly visible in the log presentation. Logarithmic presentation of a spectrum is advisable when its dynamic range is so large that small but significant peaks can be "lost in the mud" of a linear scale. The logarithim is, of course, an implicit part of an absorbance spectrum, the software for both being essentially identical. The logarithmic presentation is also appropriate to spectra taken with constant signal-to-noise ratio.

Peak detection and printout as shown in Fig. 9 are essential in identifying unknown spectra with those in a spectral library.

Although a standard scheme for so doing has not, as yet, been agreed upon, it is evident that it will be based on at least

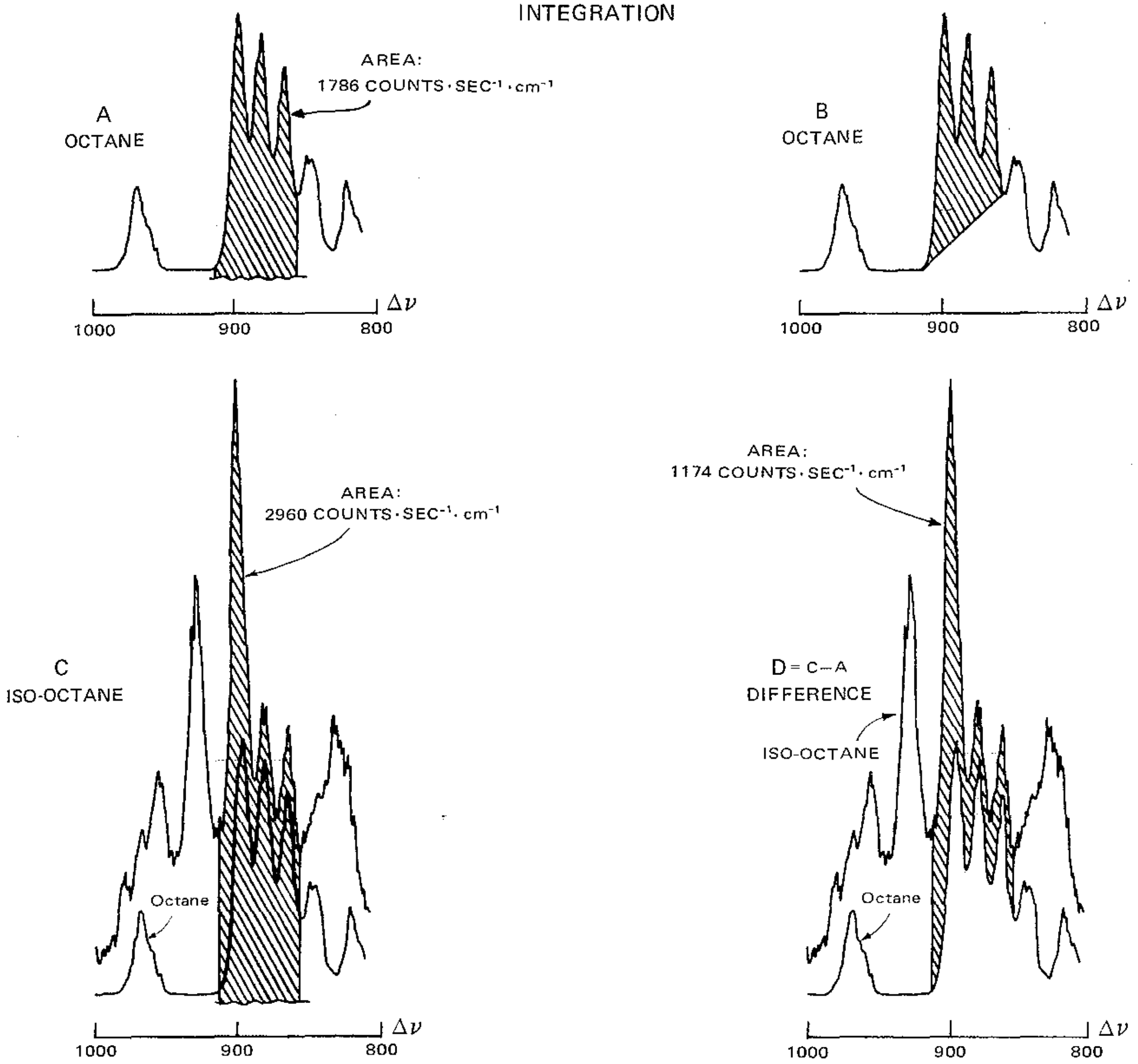

Fig. 10 Integrating the areas under the peaks and subtracting or ratioing them reveal the relative strengths of two related spectra.

three of the most intense peaks in the spectrum of the particular compound. The question is, which are the most intense peaks? Should the criterion be peak height above background or absolute intensity? Note, for example, the 11620 and 11580 cm^{-1} lines; although the absolute height of the former is smaller, its relative height above background is actually greater.

Noise peaks represent another potential source of confusion. But the software is able to cope with both of these. Smoothing is incorporated automatically to avoid fixating on a single noise spike. And detecting a real line, otherwise hidden in a valley or looking like a shoulder on a steep incline, can be enhanced by weighting the peak-recognizing algorithm with the second derivative; it is well recognized that the second derivative of a line is independent of whether the line is above a zero baseline, on the steep slope of an interfering signal, or on a high background plateau.

The effect of background can also be allowed for when computing the integrated intensity of a line or group of lines. After a survey scan and a preliminary smooth, the wavelength limits which just bracket the feature of interest can be entered in an "INTEGRATE" command. Numbers representing two different integrals are then printed out: the area including background as shown in Fig. 10A and 10C; and the area above the line connecting the intensities at the bracketing wavenumbers, as in 10B.

When comparing two related spectra, it is not necessary to perform two separate integrations. One command can call for the integral of the difference or ratio between two spectra, as illustrated in 10D, which represents the difference between 10C and 10A.

We are not stopping abruptly. The computer is becoming an accepted component of a Raman system and hardware improvements will continue to be made to its full advantage. Motorized slits, sample handlers, automated filter inserters are examples. Probably even more significant will be the projected improvements in software. Currently, we are working on deconvolution to distinguish between two or more overlapping Raman features. An automatic radiometric correction is next planned so that relative line intensities will be independent of the measuring system. This will facilitate retrieval of spectra from libraries as well as provide absolute intensity information.

But, for the most part, the work ahead lies in uncharted territory. As researchers involve themselves with ever-tougher problems, many solutions are bound to be feasible only through computer analysis and manipulation of data. We anxiously await these people-to-people interactions so we can get on with our people-to-computer interactions.

The last issue of THE SPEX SPEAKER invited reader comments. Since there have been just six responses we are printing each of them here.

23 September 1974

To the Editor:

I have just read your June 1974 issue "Society Discovers Signal-to-Noise", with its review of the global environmental problems that face us. The catalogue of ills is all too familiar, but you have put them together in a concise and convincing fashion, and argued persuasively for responsibility of science-trained individuals to aid in the process of enhancing society's signal-to-noise. What is particularly refreshing however is to see this perspective advanced in an industrial house organ. I don't recall any precedent for it. You deserve congratulations and thanks for your courage in putting yourself on the line in this fashion.

I imagine that most scientists reading your analysis would agree with your diagnosis, but would express demoralization and resignation with regard to your solution, i.e. getting more scientists involved in societal problem solving. It is abundantly clear that we need many more sharp-minded scientifically trained people to solve these problems, at the same time that we face a "glut" of Ph. D.'s. Society seems to be totally out of kilter in this, as in many other regards, and the problem, as usual, is primarily economics. Who will provide the salaries and resources to get on with the job? We scientists certainly don't have the wherewithal among ourselves. Government is pre-occupied with balancing the budget to curb inflation, and is not looking for major new ventures. If we rely on industry to finance the public interest, I fear we shall wait for a long time (unless SPEX SPEAKER is a harbinger of a radical new departure). Should we perhaps all push for conversion of the oil and mineral "depletion" allowances into a fund for environmental problem solving?

It won't be easy getting more "hands on deck", but perhaps if more of us follow SPEX SPEAKER's example and discuss the issue openly, we may overcome our demoralization and even come up with some good ideas.

Sincerely,

Thomas G. Spiro, Professor

Princeton University
Department of Chemistry
Princeton, N.J. 08540

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29 August 1974

To the Editor:

I enjoy reading your articles in the SPEX SPEAKER. I think the one on "Society Discovers Signal-to-Noise" is particularly good.

Sincerely,

Bill Bozman

National Bureau of Standards
Washington, D.C. 20234

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30 August 1974

To the Editor:

I was very pleased to read the article "Society Discovers Signal-to-Noise" in the June 1974 issue of the SPEX SPEAKER. I would like to send copies to some of my colleagues and to reference the paper, but no author is named. Could you send further information to me? Are reprints available?

Sincerely,

G. J. Zissis, Chief Scientist

E.R.I. of Michigan University
Ann Arbor, Mich. 48107

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29 August 1974

To the Editor:

The June, 1974 issue of the SPEX SPEAKER is at hand. In view of your sudden concern for the utilization of non-renewable resources, you should cease forthwith publication of your monthly bulletin.

Your article, "Society Discovers Signal-to-Noise", contained comments on energy and automotive pollution which were laughable at best, and cruelly misleading at worst. Your Elders of Zion approach to "the Atomic Energy Commission and the reactor industry, both of which are stanchly committed to present nuclear technology by powerful financial ties" deserves the contempt it will surely receive. It is obviously no use to describe to you the laudable personal qualities of the men of industrial, government, and university life who have reluctantly and dispassionately concluded that the fission reactor is our best bet for the foreseeable future. It may be more meaningful to people like you that countries east of the line between Stettin and Trieste have reached the same conclusion. They are luckier than we are in some respects. They don't have Goffmans, Sternglasses, Naders, Roismans, et alia ad nauseam. As a consequence, Russian power reactors do not have super-redundant super-safety gadgetry; their cost does not include the exorbitant legal fees, court expenses, and prolonged capital interest charges arising from bouts with the antirationals who thwart our power programs.

If bias and vested-interest is your chief concern, I, for one, find it intriguing that you fail to view with equal suspicion the gaggle of intervenors who have made a well-paying legal industry out of obstruction of the public utilities, and harassment of the chemical and fuel industries.

Let's stop the nonsense about motives, cui bono, etc. and deal with the facts of the case. The probability of a serious reactor accident, fuel diversion, fission product loss, etc., is equivalent to that of a Metroliner running wild out of Penn Station and up Broadway at rush hour. The environmental damage associated with digging up the state of Wyoming and sending it through a smokestack is somewhat greater than that associated with the mining of a few tons of uranium. The probability of genetic damage, death, injury, disfigurement, etc. due to smoking, bike riding, spinach (oxalic acid), chlorinated water (a mutagen), mustard (another mutagen) overwhelms those associated with all aspects of fission power.

Truly, I find your presentation unfit for a lay audience and an outright insult to the scientific community.

Do you really believe you have provided us with more signal than noise? I don't. Unless you can provide this reader with hard scientific information in a dispassionate manner, please spare yourself the trouble and our society the cost of sending me your bulletin.

J. Silverman, Professor

Department of Chemical Engineering
University of Maryland
College Park, Md. 20742

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29 August 1974

To the Editor:

I am writing to simply say that I enjoyed your editorial in the June issue of the SPEX SPEAKER. I also edit a journal in optics, for which I write a monthly editorial, and now and then I try to venture into practical topics; but I have ordinarily just nibbled on small matters: you have tackled the whole major area of public interest science! Good for you, and I hope you can keep it up.

Sincerely,

John N. Howard, Editor, Applied Optics

Chief Scientist, AFCRL
Bedford, Mass. 01730

To the Editor:

29 August 1974

I found your lead article in the most recent SPEX SPEAKER (Vol. 19, No. 2, June 1974) on "Society Discovers S/N" to be most interesting. I would like to use it in my physics courses when we get to environmental impact.

I request that you send me 40 copies or reprints of the article, and bill me for the charges.

Sincerely,

Nelson Fuson, Professor of Physics

Fisk University
Nashville, Tenn.

WESTERN REGIONAL OFFICE: 3246 McKINLEY DR., SANTA CLARA, CA. 95051 408/246-2333

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