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Analog Spectrophotometers in the Digital Age: Data Acquisition on a Budget

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It is scarcely possible to go into a modern laboratory and not find computers hard at work. Computer data processing enables us to perform numerous helpful operations otherwise practically impossible: baseline correction, digital differentiation and integration, convolution, to name the few *(1–3)*. Acquiring data from instrumentation, archiving the recorded spectra, and preparation of reports using appropriate software are common laboratory tasks.

There are numerous new UV–vis and IR (mostly FTIR) spectrophotometers of high and intermediate levels of resolution that can easily perform the above-mentioned operations. Significant cost of such systems often prevents them from appearing in the undergraduate laboratory. On the other hand, low resolution systems (1–5 nm for UV and 10 cm^{-1} for IR), which are still expensive, often cannot provide enough resolution for some interesting laboratory experiments.

At the same time older models of scanning UV–vis and IR instruments can show good resolution, stability, and accuracy, thus performing better than some newer computerized systems. Usually the older models are able to record a spectral area of interest in several minutes. This is compatible with the time necessary for sample preparation and data processing. The limiting step is the conversion of the analog output signal coming from such an instrument into a digital format. Considerable cost of high performance analog-to-digital converters greatly limits their use for upgrading the old instrumentation.

Certainly, the instructor can build a homemade data logger. For example, a simple design including an educational Stamp 2 microprocessor and a 12-bit analog-to-digital converter is described in detail in *(4, 5)*. The use of a Visual Basic program and a 14-bit data acquisition card to interface scientific instruments to a personal computer were demonstrated in ref *6*. An even simpler solution is to use an off-the-shelf device. Two types of 12-bit data loggers, LabPro (Vernier Inc.) and digital multimeters with an RS-232 interface, are commercially available. LabPro is widely used in high school and undergraduate laboratories *(7)*. Some analog spectrophotometers, such as a Spectronic 20, can be connected to the computer through the LabPro computer interface. Digital multimeters are common maintenance tools in the instrumental laboratory. The interfacing of Metex model M4650CR and Radio Shack model 22-168 multimeters to personal computers and to an Apple Newton PDA handheld computer was described in ref *8*. A Lego spectrophotometer interfaced to a digital multimeter was recommended in ref *9*. The use of a data logger in conjunction with an oxygen electrode to monitor the generation of oxygen in photosynthesis was demonstrated in ref *10*.

In this article we would like to share our experience with interfacing various spectrometers with analog output to a personal computer running Microsoft Excel in the Windows environment.[1]

Experimental

Data Logger Setup

Numerous multimeters with serial interface are available. The simplest available multimeter with the RS-232 serial connection, Craftsman model 82324 (the same device as RadioShack 22-805 or Metex ME-11) was used. Only two modes, 0–4.000 V and 0–400.0 mV, were employed. Other digital multimeters, the Craftsman 32257 and RadioShack 22-812, were also tested; while showing similar performance, they require different software for data acquisition *(11)*. The multimeter performs 1–2 measurements per second (actual time between measurements can be changed by changing the delay time). The opportunity to see the actual voltage readings before logging the data into computer is very helpful when adjusting the system and troubleshooting.

A more expensive and advanced LabPro with or without the auxiliary amplifier was employed with the same instruments with the rates of 5–20 measurements per second.

Programming Tools

Data Collection Program

At this step, we want to collect the data in a digital format and to store them in the computer. A simple “radar”’ graphic window is helpful to visualize this process. Practically all digital multimeters with PC interface come with some software for data collection. LabPro comes with a well-developed interface program, Logger Pro. Nevertheless, it is convenient to make a custom program that may include peculiarities of the particular instrument. Writing such program is outlined in ref *12*. Very helpful code for the interface writing can be obtained from refs *11–14*. The data collection program can be opened from the Excel environment; an alternative approach is simply open it in a separate window along with Excel file. Several examples of code for digital multimeters and for LabPro are presented in Supplemental Material.W

Excel Interface

We use Microsoft Excel as an environment for our project. Excel is often considered to be one of the most easily learned tools for numerical data analysis *(2, 3, 15)*. It is widely available as it is a part of Microsoft Office. A Visual Basic macro first runs the data logger program. After the data have been acquired and written in the file (e.g., "test.dat"), they can be transferred into Excel spreadsheet. The essential code that does this is shown in Table 1. In the Excel spreadsheet, the raw data are calibrated using usual Excel functions to form a spectral data file.

In most of our laboratory experiments we use Excel simply to visualize the data. The instructor may want to preconfigure the plot in advance to make it attractive (for example, to make appropriate axes and gridlines) and to save laboratory time. Numerous uses of Excel in spectral data processing are given in refs *2, 3*. In our setup we also add a macro that saves the processed data in ASCII format making it available for database processing software. Some of the examples are presented in Supplemental Materials.[W]

Commercial software available to facilitate the importation of experimental data directly from a serial port into Excel should be mentioned *(16)*.

Spectrophotometer Setup

A Beckman DU-G spectrophotometer was selected as an example of a UV–vis instrument. A Beckman Acculab 4 scanning IR spectrometer was used for measurements in the infrared region. Both instruments have an analog output for an external chart recorder. Output voltage is 0–100 mV and 0–1 V, respectively. For UV–vis instruments, scanning rates of 10 nm/min and 60 nm/min were used. The IR spectrum measurements were performed in 7 min mode (that is, 7 min per spectrum with different rates for 2000–4000 cm^{-1} and 600–2000 cm^{-1} ranges). We have also tested PerkinElmer Lambda 3 and PerkinElmer 1420 IR spectrometers.

Results and Discussion

UV–Vis Spectrophotometer

Even at a high scanning rate (60 nm/min) the multimeter data logger produces one data point per nanometer. This resolution is enough for most common absorption bands. As a crucial test of the system performance, the visible spectrum of holmium perchlorate standard solution was measured (Figure 1). The results are compared with the readings taken by diode array HP 8453 instrument using the similar solution. The positions of the sharp Ho^{3+} peaks and their shape in these two spectra practically coincide. The data logger scan shows insignificant (if any) memory effects. Thus, the spectrophotometer-DMM-PC system does not corrupt the data and can produce a high quality spectrum.

Higher resolution of six data points per nm can be achieved at a slow rate (10 nm/min). This resolution is seldom necessary for the molecular spectroscopy in solutions; the benzene vapor at 240–280 nm (Figure 2) is shown as an example. This spectrum is often discussed in the spectroscopy textbooks or used as a test of instrument performance. Some further improvement can be achieved using higher sampling (Figure 2, curves A and B). The fine structure of the benzene spectrum cannot be observed using the HP 8453

Table 1. Code To Transfer Data into an Excel Sheet

Code	Function
Open "test.dat" for input As #1	Opens the ASCII file
n = 1	
Do While Not EOF(1)	Starts loop till the end of file
Input #1, number, absorbance	Reads data from file
Worksheets("RawData"). Cells(*n*, 1).Value = number	Writes the number in column A in sheet "RawData"
Worksheets("RawData"). Cells(*n*, 2).Value = absorbance	Writes the measurements in column B in "RawData"
n = *n* + 1	Counts number of the data processed
Loop	End of the loop
Close #1	Closes the ASCII file

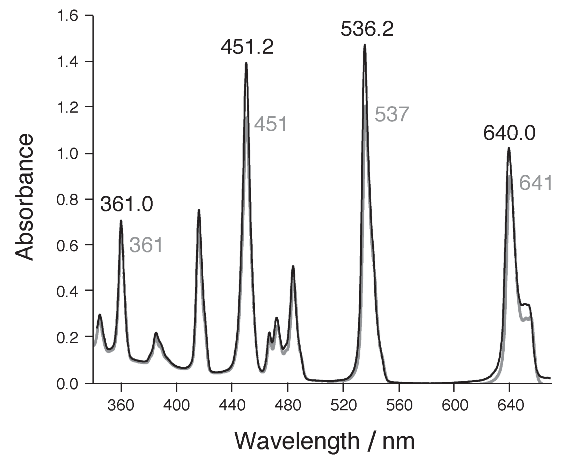

Figure 1. Holmium perchlorate spectrum in the visible region measured using Beckman DU-G with multimeter data logger (scan rate 60 nm/min, 1 measurement per second) (black line) and HP-8453 (gray line). The solution mimics the NIST SRM No.2334.

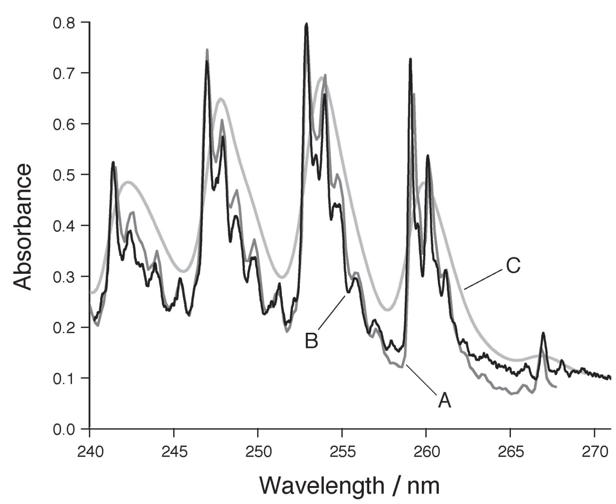

Figure 2. Benzene vapor spectrum measured using Beckman DU-G scanning spectrophotometer with (A) LabPro data logger (scan rate 10 nm/min, 10 measurement per second), (B) multimeter data logger (scan rate 10 nm/min, 1 measurement per second), and (C) HP-8453.

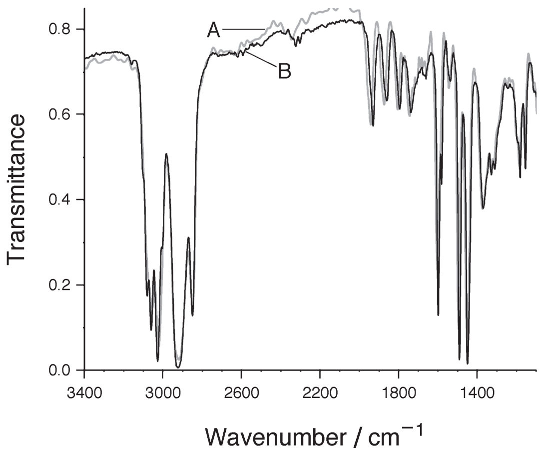

Figure 3. IR spectra of polystyrene film measured using Beckman Acculab 4 with (A) multimeter data logger (7 min per scan, 1 measurement per second) and (B) LabPro data logger (3 min per scan, 10 measurements per second). The film was a PerkinElmer standard similar to NIST 1921a.

(curve C).

The stability of readings in the system with the data logger is well within the limits observed for common UV–vis spectrophotometers. The standard deviation of baseline readings was around $\pm 4 \times 10^{-4}$ for both our system and OceanOptics PC-2000 while it was much lower on the diode array HP 8453 ($\pm 5 \times 10^{-5}$). Therefore, the data logger does not introduce extra noise into the measurements.

IR Spectra

To test the performance of the infrared scanning spectrophotometer with the data logger, we employed a polystyrene standard film. With the multimeter data logger, the distance between the data points was 12 cm^{-1} in 2000–4000 cm^{-1} range and 7 cm^{-1} in 600–2000 cm^{-1} range. The resulting spectra are in a reasonable agreement (± 3 cm^{-1}) with the NIST standard. From our experience, the actual readings made by students may deviate to a larger extent but still will not exceed 8–10 cm^{-1} even at the high scan rate (7 min for the 600–4000 cm^{-1}). Slower rates lower the error to the level of 1–2 cm^{-1}, which is the limit of the instrument itself. For example, vibrational–rotational spectra *(17)* of HCl and DCl can be recorded. The use of LabPro with data rate of 5–10 measurements per second significantly improves the picture, and 5–8 cm^{-1} resolution can be achieved even in 3-min scan (Figure 3). It is convenient to calibrate the system directly in the Excel file using the polystyrene standard.

The instruments described above were used for various laboratory experiments in instrumental analytical chemistry and in organic chemistry laboratories at the State University of New York, College at Buffalo in 2001–2002. The original spectra as well as short lab instructions are presented in Supplemental Materials.[W]

Conclusions

The addition of a simple data logger to an “obsolete” scanning spectrophotometer can transform it into a contemporary computerized instrument. This low-cost data acquisition solution (less than $100 and five minutes to set up) is a useful replacement of a chart recorder for various UV–vis and infrared scanning spectrophotometers. The proposed data loggers do not compromise the quality of the measurements. Embedding the data in an Excel worksheet makes it a convenient tool for a wide range of data processing applications. All the software in use is familiar to most chemistry students.

Acknowledgment

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[W]Supplemental Material

Several examples of code for digital multimeters and for LabPro are available in this issue of *JCE Online*.

Note

1. This material was presented in part at 224th ACS National Meeting in Boston, MA, August 2002.

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