VERNIER SOFTWARE
SPECTRO PROGRAM
WITH TI Graphing Calculators and TI CBL, CBL 2 or LabPro

OVERVIEW

This document briefly describes the use of a program, SPECTRO.??p, that supports the use of the ThermoSpectronic Spec 20 and Spec 20D spectrophotometers with a TI graphing calculator and the CBL, CBL 2 or LabPro interface. The spectrophotometer is connected to the interface with a serial cable and a CBL-DIN adapter. The spectrophotometer must have a 6-pin female connector (for a 6-pin Jones Plug) on the bottom of the spectrophotometer. The serial cable (SPC-DIN, $25.00) and DIN adapter (CBL-DIN, $5) are available from Vernier.

The program provides four data-collection modes: 1) monitor the absorbance, 2) collect and graph absorbance *vs*. time data, 3) collect and graph absorbance *vs*. concentration data, and 4) collect and graph absorbance *vs*. wavelength data. The program can record both absorbance and percent transmittance, but wavelength must be typed in as a prompted input.

GENERAL DESCRIPTION OF THE PROGRAM

The following general description applies to the use of this program on the TI-83 Plus calculator. For specific help in executing programs on the calculator, refer to the manual. To begin, run the SPECTRO program. After an introductory screen, the following main menu will appear:

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*MAIN MENU*
1:SET UP PROBE
2:COLLECT DATA
3:VIEW DATA
4:QUIT
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The first option, SET UP PROBE, allows you to calibrate the spectrophotometer. This program assumes that the spectrophotometer is connected to channel 1 of the interface. Calibrate the spectrophotometer at the 0% transmittance without a cuvette and 100% transmittance with a blank cuvette. After calibration, you will return to the MAIN MENU to begin data collection. After selecting option 2, COLLECT DATA, the following menu will appear:

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DATA COLLECTION
1:MONITOR INPUT
2:ABSORB VS TIME
3:ABSORB VS CONC
4:ABSORB VS WAVE
5:RETURN
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The MONITOR INPUT option allows you to use the calculator and CBL, CBL 2 or LabPro to monitor the absorbance. The purpose of this option is to view data at 1.0 second intervals. No data is stored.

The ABSORB VS TIME option allows you to graph absorbance as a function of time. You will be prompted to enter the time between samples, in seconds. The sample time can be in the following range of values: 0.000165 to 0.2 seconds or 0.25 to 16000 seconds. After the sample time is entered, you will be prompted to enter the number of data points to collect. After the experiment is run, the time is stored in list L1, absorbance in L2 and transmittance in L3.

The ABSORB VS CONC option allows you to collect absorbance values as a function of concentration (Beer's law). The interface and calculator collect absorbance data for each sample while you manually enter the sample's concentrations. As the experiment proceeds you will monitor the absorbance for each sample. If you are using a CBL interface watch the CBL screen for % transmittance and press the [TRIGGER] button on the CBL when it has stabilized. If you are using a CBL 2 or LabPro interface watch the calculator screen for % transmittance and press the [ENTER] key on the calculator when it has stabilized. Follow the instructions on the calculator screen to record the data and then type in the concentration. This process is repeated for each new sample. The concentration will be stored in list L1, the absorbance in list L2, and % transmittance in L3.

The ABSORB VS WAVE option allows you to collect absorbance values as a function of wavelength. The calculator and interface collect absorbance data for the sample at different wavelengths while you manually enter each new wavelength. With each new wavelength setting, you will recalibrate the spectrophotometer for 100% transmittance by placing a blank in the spectrophotometer, set the spectrophotometer to 100%, and press the [TRIGGER] button on the CBL or the [ENTER] key on the calculator when the signal has stabilized. You then place the sample in the spectrophotometer and again press either the [TRIGGER] button on the CBL or the [ENTER] key on the calculator when the reading stabilized. You will then manually type in the wavelength. This process is repeated for each new wavelength. The wavelength will be stored in list L1, the absorbance in list L2, and transmittance in L3.

The third option on the main menu, VIEW DATA, exits you from the program allowing you to view, edit and analyze the data stored in the lists. Press the [STAT] button on the calculator and choose the Edit option to view the lists.

Option four, QUIT, will exit the program without resetting the interface.

POSSIBLE ACTIVITIES

Here are some suggested experiments that can be performed with this program.

1) Standard solutions that are 0.1, 0.2, 0.3 and 0.4 M $CuSO_4$ will yield a good Beer's law curve using a wavelength of 630 nm with a spectrophotometer. Or prepare a stock solution by adding 10 g of NH_4NO_3 to 10 mL of 0.1 M $CuSO_4$ and 90 mL of 0.20 M NH_3 (forms the $Cu(NH_3)_4^{2+}$ complex ion) and dilute to obtain standard solutions.

2) A less expensive alternative to using the solutions above is to prepare solutions using food coloring. Very good Beer's law curves can be obtained using these solutions. Add about 6 drops of red, blue or green McCormick brand food coloring to 1 liter of water. The red solution can be analyzed at a wavelength of 510 nm with a spectrophotometer. With green food coloring, use a wavelength of 600 nm and use a wavelength of 620 nm for the blue solution. Since the actual concentration of the solutions will not be known, refer to the original solution as "100%" and then dilute to 80, 60, 40, and 20%.

3) Rate law determination can be done when 2.0 X 10^-5 M crystal violet reacts with 0.10 M NaOH. Combine equal volumes of these solutions (10 mL

of each works fine). Collect absorbance data at a wavelength of 565 nm for three minutes. Analysis of absorbance *vs*. time, 1/(absorbance) vs. time, and ln(absorbance) vs. time graphs show the reaction to be first order with respect to crystal violet. The crystal violet solution is prepared with 0.016 g crystal violet in 2 L of solution. Sodium hydroxide solution uses 4 g of NaOH per liter of solution.

4) To determine the concentration of an ion in a colorless solution using a spectrophotometer, an agent must be added to the solution to yield color (such as a colored complex ion) or turbidity through the formation of a precipitate. The assumption is that the intensity of the color (and its resulting ability to absorb light) is proportional to the concentration of the ion in solution. Hach Company markets pre-massed pillows for analysis of such ions as nitrate (NO_3^-), sulfate (SO_4^{2-}), phosphate (PO_4^{3-}), water hardness (Ca^{2+}), or dissolved oxygen. A wavelength and colorimetry method is recommended for each of these ions. Pillows are available for various concentration levels (i.e., 1-100 mg/L, 1-10 mg/L). Try adding these pillows to samples of water collected near your school and analyze for ion concentrations using your spectrophotometer. You may obtain a Hach Catalog by writing to: Hach Company, P.O. Box 389, Loveland, CO 80539. Or call: 1-800-227-4224. Or visit: www.Hach.com

5) Test for turbidity of stream samples using standard methods with a spectrophotometer. Devise a method for determining the settling rate of sands of different coarseness.

6) An absorption spectrum can be made for nearly any solution using the absorbance vs. wavelength experimental mode of this program. Place a sample of a solution in a 13 X 100 mm spectrophotometer test tube. You will first be instructed to zero-calibrate the spectrophotometer by removing the sample and adjusting the zero control to read 0.0% transmittance. Then you will be instructed to change the wavelength on the instrument, calibrate at 100% transmittance using a blank, insert your sample, and collect the absorbance data. You will then have to type in the wavelength reading shown on the spectrophotometer. You can repeat the process with as many wavelengths as you wish. When you have finished collecting data, you can view a graph of absorbance *vs*. wavelength.

7) It is also possible to produce an absorption spectrum for photosynthetic pigments, such as chlorophyll *a*, chlorophyll *b*, lutein, or beta-carotene. Following their separation and extraction using paper chromatography, each pigment is eluted from the chromatography paper using acetone. The resulting filtered solution can be read at wavelengths from 400 to 640 nm, with the SPECTRO Program, using acetone as a blank. The presence of any of the chlorophylls or carotenoids can be determined by examining the wavelength value of peaks in the spectrum.

8) You will find other experiments in these books:

Holmquist, Dan and Volz, Don. “Chemistry with Computers”. Vernier Software.

Holmquist, Dan and Volz, Don. “Chemistry with Calculators”. Vernier Software.

Holmquist, Dan; Randall, Jack; Volz, Don. “Chemistry with CBL”. Vernier Software.

“Educational Manual for the SPECTRONIC 20 and 20D Spectrophotometers”, Milton Roy Company.

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