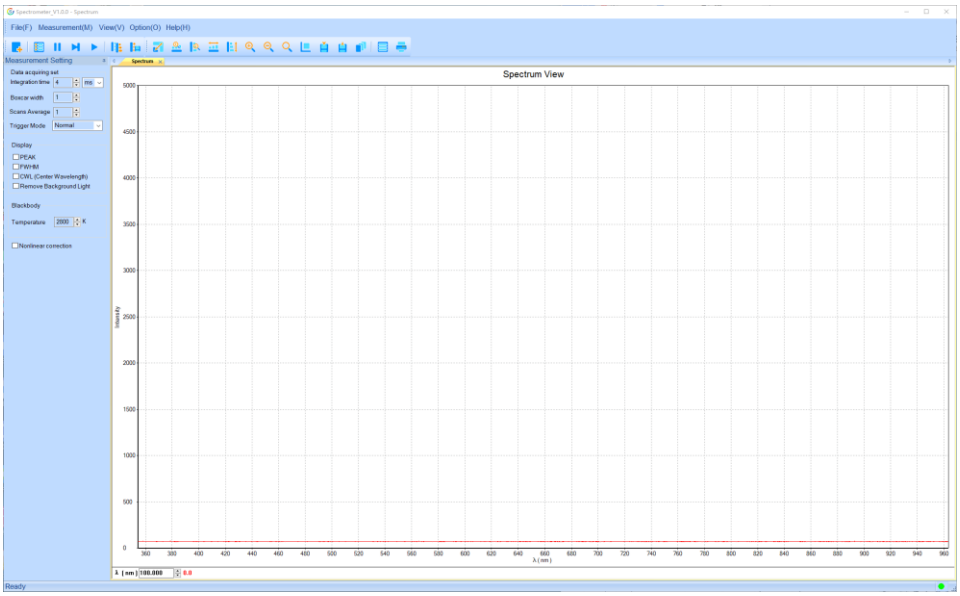
User manual for Spectrometer Basic Software

Version 1.0

I Use of Windows version

a) Click  to enter the special software of the spectrometer, and enter the home interface



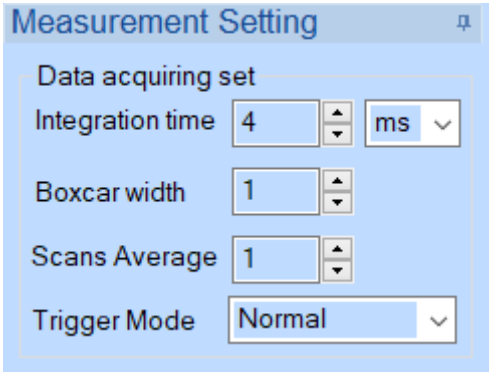
 Shown in the lower right corner of the figure above means connected。

b) Introduction to interface functions

Icon function ：

	New create		Setting
	Stop		single-step
	Start		Save reference spectrum
	Save Dark		Restore
	X-axis magnification		Y-axis magnification
	X-axis adaptation		Y-axis adaptation
	Enlarge		Reduce
	Local Scale		Coordinate setting
	Import data		Export data
	Data management		Add Table View
	Print		

Measurement Setting：



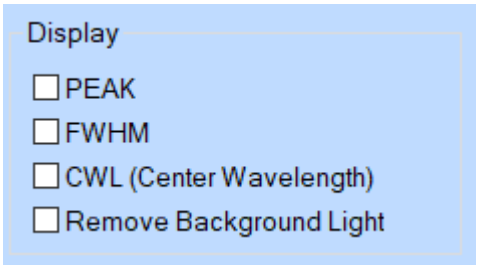
Integration time: The greater the integration time, the stronger the signal.

Boxcar width: The larger the set smoothness value, the smoother the waveform.

Scans Average： Take the average of multiple measurements.

Trigger Mode： Trigger data collection

Display：



PEAK： Display crest information.

FWHM： Display the wave peak half-width information.

CWL： Displays the center wavelength information.

Display the spectrum after deducting the dark light spectrum: display the spectral data after deducting the background light.

Color temperature: the relevant color temperature of the light source

Ⅱ Typical experimental cases Determination of KMnO4 solution concentration

Purpose

1. Determine the absorbance of KMnO4 solution at a specific wavelength and obtain the concentration - absorbance standard curve of KMnO4solution.
2. Determine the absorbance of the unknown KMnO4 solution and calculate the concentration of the unknown solution according to the standard curve.

Experimental principle

Colored material solution can selectively absorb part of the energy of visible light and present different colors. The absorption spectrum of substances can be formed by absorbing some wavelengths of light emitted by the light source. Due to the different molecular structures of substances and their different absorption abilities to light, each substance has a specific absorption spectrum, and under certain conditions its absorption degree is proportional to the concentration of the substance. The qualitative or quantitative analysis of different substances can be carried out by using this absorption characteristics of substances.

The color depth of the material solution depends on the intensity of the incident light, the concentration of the colored material solution and the thickness of the liquid layer. When a beam of monochromatic light irradiates the solution, the stronger the intensity of the incident light, the greater the concentration of the solution, the thicker the liquid layer, and the more light absorption of the solution. The relationship between them conforms to the quantitative law of light absorption of substances, namely, Beer-Lambert Law. This law is the theoretical basis for the quantitative analysis of substances by spectrometer.

Lambert-Beer law： $A = -\lg(T) = \epsilon bc$

A : absorbance
T ： transmissivity
b ： Liquid layer thickness (optical path length), usually in cm
c ： Molar concentration of solution， unit mol/L
ε ： Molar absorptivity， unit L·mol/cm

➢ A is proportional to molar absorption coefficient, optical path and molar concentration of solution;

➢ A is related to the wavelength of the incident light and the material passed by the light. As long as the wavelength of the light is fixed, the absorption coefficient of the same material will not change.

Experimental equipment

0.001g precision scale, 1 beaker, 1 stirring rod, 1 1000ml volumetric flask, 5 100ml volumetric flasks, 1 pipette 1ml, 5ml and 10ml each, 1 spectrograph, 6 colorimetric cells

Main equipment

Step

1. **Solution preparation**

(1) Weigh 1.58g of KMnO4 solid, put it in a beaker, stir and dissolve it with distilled water, use a 1000ml volumetric flask to volume to the scale, and mix well. The concentration of the solution is 0.01 M.

(2) Take five clean and dry 100ml volumetric flasks, use a pipette to take 1.0, 3.0, 5.0 and 9.0 ml of the above solutions, put them into four volumetric flasks respectively, add water to dilute to the scale, shake well, and obtain the KMnO4 solution concentration of $1 \cdot 10^{-4}$ M, $3 \cdot 10^{-4}$M, $5 \cdot 10^{-4}$ M, $9 \cdot 10^{-4}$ M

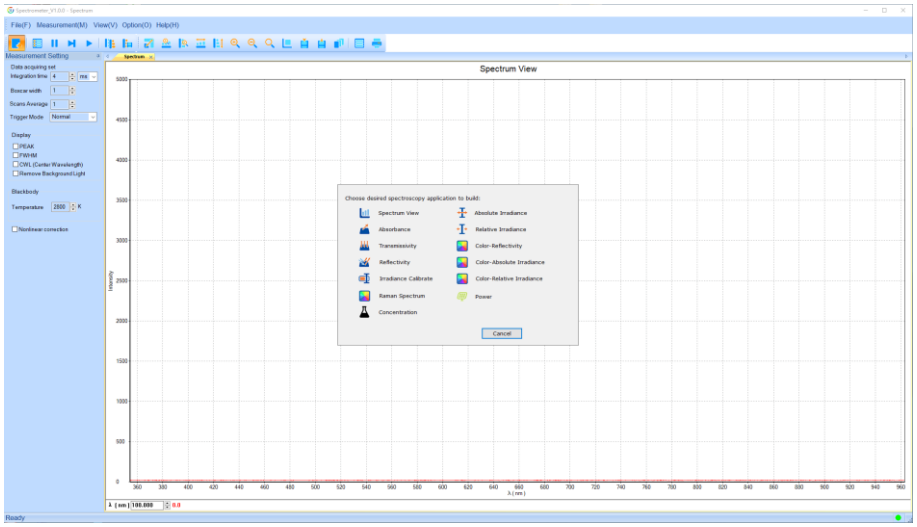
(3) Prepare solution of unknown concentration

(4) Prepare distilled water as reference sample.

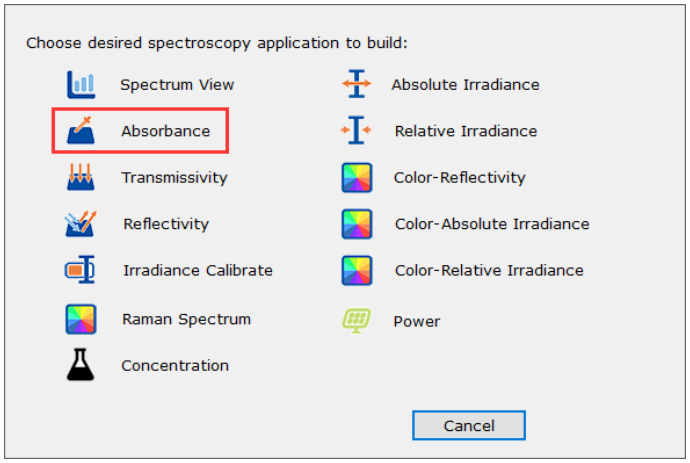
2. Connecting software

(1) Connect the spectrometer with the computer, open the software, and the button in the lower right corner will turn green, then the instrument connection is completed.

(2) Click the "New Measurement" button on the toolbar to open the new test interface.

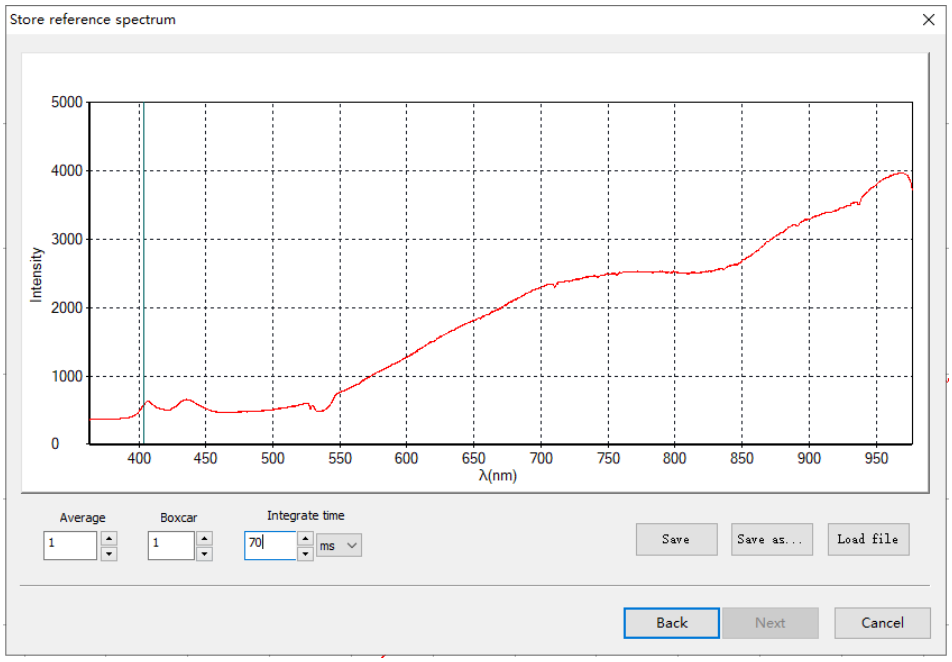


(3) Click the "absorbance measurement" button to start the absorbance test and pop up the test wizard.

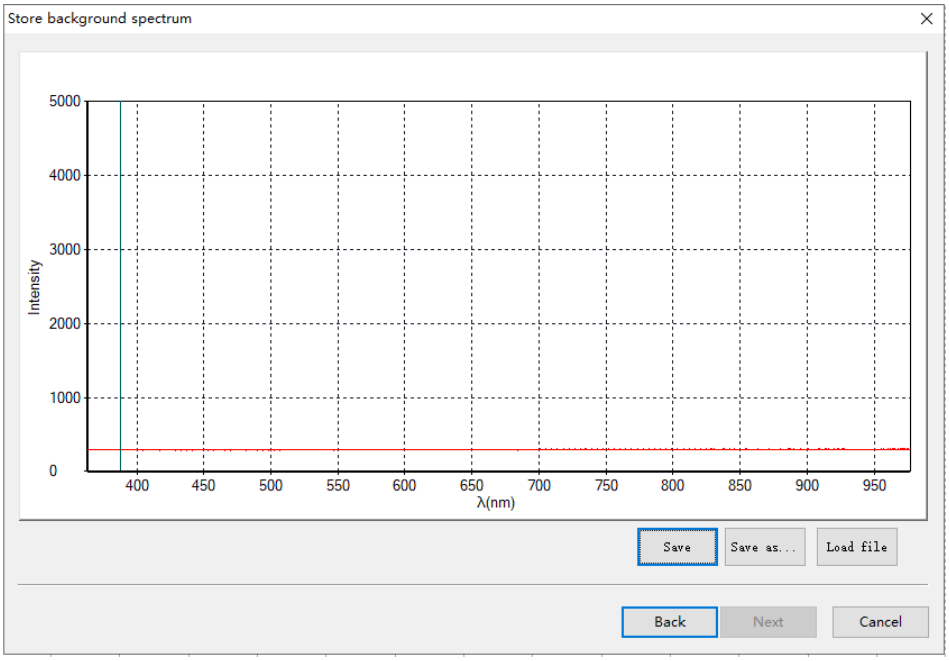


(4) Calibrate after light absorption, add 3/4 of distilled water solution into the cuvette and put it into the cuvette tank.

(5) According to the test wizard, adjust the integration time (make the peak value of the highest wave peak at 80% of the saturation intensity), the smoothing coefficient and the average number of samples (when there is large noise or the waveform changes greatly, you can set the appropriate average number of samples to reduce the noise and obtain stable data). After the modification, click the "Save" button to save the reference spectral data, and then click the "Next" button.



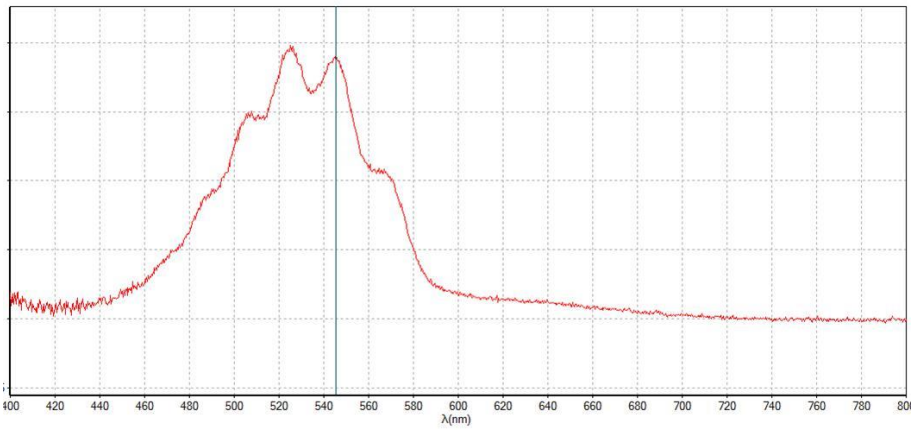
(6) Block the light source (insert the black plug end of the optical fiber into the cuvette slot to block the light source), so that the light from the light source cannot enter the spectrometer, and then click [Save dark spectrum] to save the background spectrum.



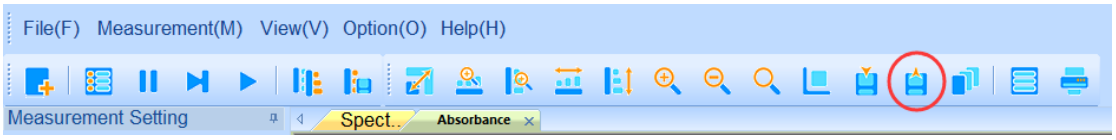
(7) Click [Finish] to end the test wizard and enter the absorbance test interface.

3. Measurement sample

(1) Use a cuvette to hold $1 \cdot 10^{-4}$ mol·L $^{-1}$ KMnO4 solution of, put into the cuvette tank for measurement. Pay attention to the same position as the reference sample and obtain the absorbance diagram as shown below.



(2) Export and save the data.



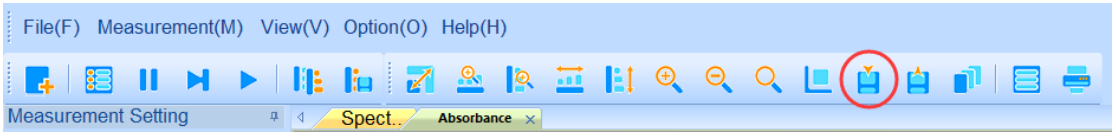
(3) Repeat steps (1) and (2) for the remaining known and unknown solutions, and the measurement is completed.

4. Data processing: determine the maximum absorption wavelength of KMnO4 solution

Determine the absorbance value A at the maximum absorption wavelength. Draw A-c curve. Calculate the concentration of unknown KMnO4 solution.

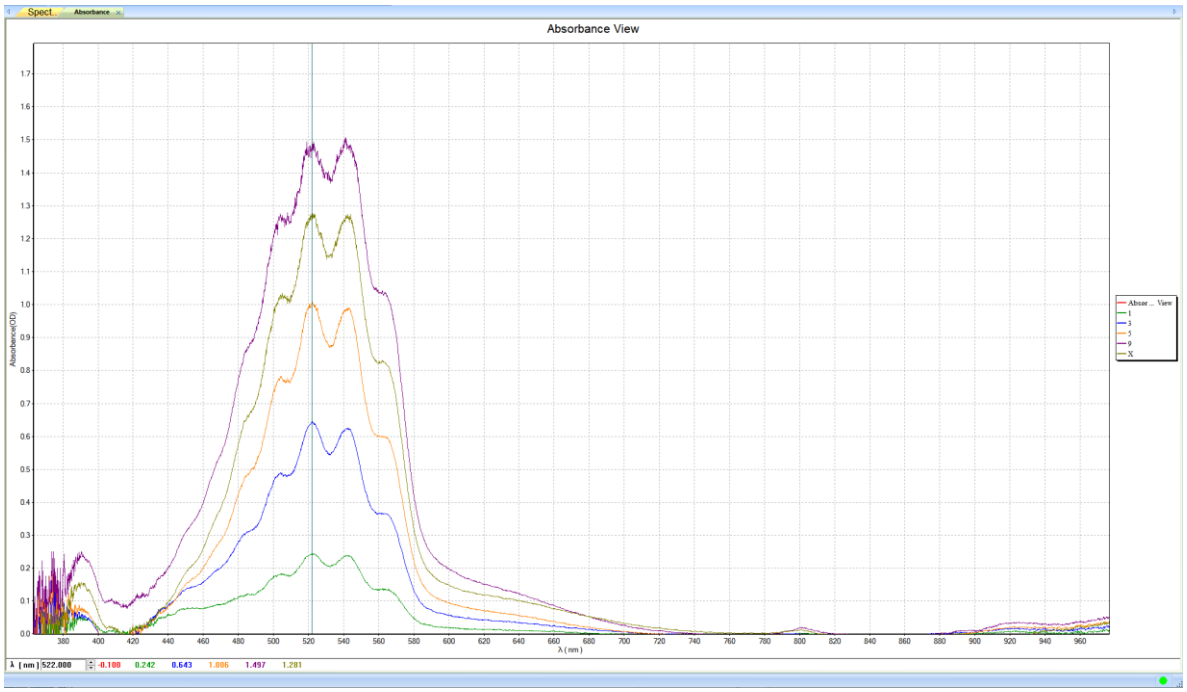
The method is as follows：

(1) Click the "Data Import" button to import all test data for analysis.



(2) From the data, we can see that the absorbance curve of KMnO4 solution has two peaks. We select the absorbance value corresponding to the maximum absorption wavelength of

22nm for data processing.

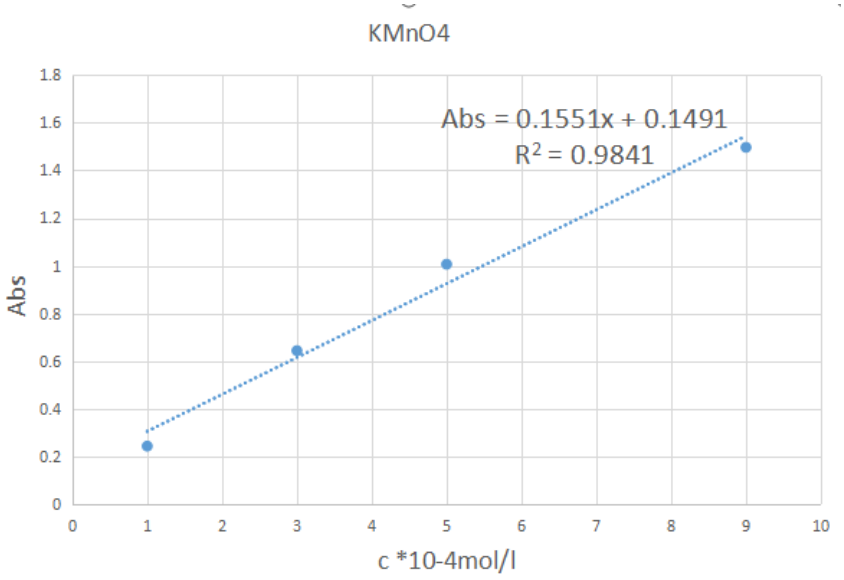


(3) The data results of absorbance A and solution concentration c are as follows:

C(mol/L)·10 $^{-4}$	1	3	5	9	X
absorbance	0.242	0.643	1.006	1.497	1.281

Fit the data in the above table

Insert a scatter chart in Excel, select the data points to be fitted, set the horizontal and vertical coordinates, check the display trend line, fitting equation, R2 (goodness of fit), and get the following.



Calculated:

X=7.30·10 $^{-4}$mol/L