Egypt.J.Chem. **Vol. 63**, No. 1. pp. 197 - 201 (2020)

Egyptian Journal of Chemistry
http://ejchem.journals.ekb.eg/

Slit Width Effect on Signal-to-noise Ratio in Spectrophotometric Measurements

Alaaeldin Abdelmageed, Essam Elmoghazy and Fatma El-Sharkawy*
National Institute of Standards (NIS), Photometry and Radiometry Division, Tersa St., P.O. Box 136, Giza, Egypt

SIGNAL-to-noise (S/N) ratio theory has proven to be useful in understanding, designing, and optimizing spectrophotometric measurement systems. Although a narrower spectral bandwidth does improve the resolution of closely spaced peaks, it also decreases the Signal-to-noise ratio. The narrowest slit width should be used that will yield an acceptable Signal-to-noise ratio. In this research, the wavelengths of peak absorbance of the holmium glass filter were determined to attain the optimum Signal-to-noise ratio accompanied with spectral bandwidths of 0.1 nm, 0.2 nm, 0.5 nm, 0.8 nm, 1 nm, 2 nm, 3 nm and 5 nm. The influence of spectral bandwidth on the Signal-to-noise ratio was by far the most important parameter affecting the location of the measured wavelengths of absorbance or transmittance of the sample.

Keywords: Spectrophotometer, Slit width, Signal-to-noise ratio, Absorbance of the sample.

Introduction

One of the most important parameters the analyst must select is the spectral slit width. It is defined as the width (usually expressed in mm) of the entrance and exit slits of a monochromator. Selecting the appropriate spectrophotometer to comply with the complex requirements of a regulated laboratory can be a daunting task. Two specifications that have become increasingly challenging are resolution and spectral bandwidth [1-6]. The slits are rectangular apertures through with light enters into and exits from the monochromator. Their purpose is to control the spectral resolution of the monochromator, that it, its ability to separate close wavelengths. The optimum slit width will be determined by the spectral characteristics of the sample and the dispersion of the instrument used (ignoring variation among detectors). Where instrument resolution is more than adequate, the Signal-to-noise ratio is maximized [7]. In order to make meaningful measurements and to be confident in the quality of the data obtained, an experimentalist must ensure using the optimum slit width with the highest signal to noise ratio [1, 7].

The true monochromatic absorbance follows the Beer-Lambert Law; the absorber has a Gaussian absorption spectrum; the monochromator has a Gaussian slit function; the absorption path length and absorber concentration are both uniform across the light beam; the spectral response of the detector is much wider than the spectral bandpass of the monochromator; a double-beam instrument design measures both sample and reference beams and both beams are subject to random and uncorrelated noise [1]. Where instrument resolution is more than adequate, the Signal-to-noise ratio is maximized. The analyst must evaluate the effect that slit width has upon resolution. Alternatively, spectral slit width provides an expedient means of expressing theoretical resolution. Many factors in instrument design influence the selection so that it is necessary for an analyst to determine the optimum slit width

---

*Corresponding author e-mail: fsharkawy_2000@yahoo.com
Received 9/7/2019; Accepted 26/8/2019
DOI:10.21608/ejchem.2019.14559.1884

for a particular analysis and instrument. Noises in the UV-VIS measurement are mainly originating from the light source and electronic components. Noise in the measurement affects the accuracy at both ends of the absorbance scale. Photon noise from the light source affects the accuracy of the measurements at low absorbance. Electronic noise from electronic components affects the accuracy of the measurements at high absorbance. High noise level will reduce the limit of detection and render the instrument less sensitive.

Experimental

UV-Vis Spectrophotometer type UV-3101 PC from Shimadzu Inc., is used [8]. It has dual light sources. A deuterium lamp is used for the UV range and a tungsten lamp is used for the visible range. The dual-beam spectrophotometer was developed to compensate for these changes in lamp intensity between measurements on blank and sample; see Fig. 1. Various factors which affect the reliability of the UV-Vis measurement were discussed [9]. To avoid errors due to spectral slit-width, when using UV-3101 on which the slit-width is variable at the selected wavelength, the slit-width must be small compared with the half-width of the absorption band but it must be as large as possible to obtain a high intensity value. The spectral bandwidth of the instrument will always be narrower than the spectral slit width. A spectrophotometer typically has two noise elements. The first element (photon or Schott noise) results from the statistical distribution of the photons emitted by a light source. It is proportional to the square root of the intensity of light. When low concentration samples with low absorbencies are measured, this element may prevent an accurate measurement of the small difference between two high light levels. The second element is inherent to the instrument electronics (detector amplifier, analog-to-digital converter, and so forth) and is independent of the intensity measured. This element becomes significant at high absorbance levels, where the sample signal is very small. It can be minimized through good design. Noise negatively affects the precision of measurements and, for any single measurement, may introduce errors inaccuracy as well [10,11].

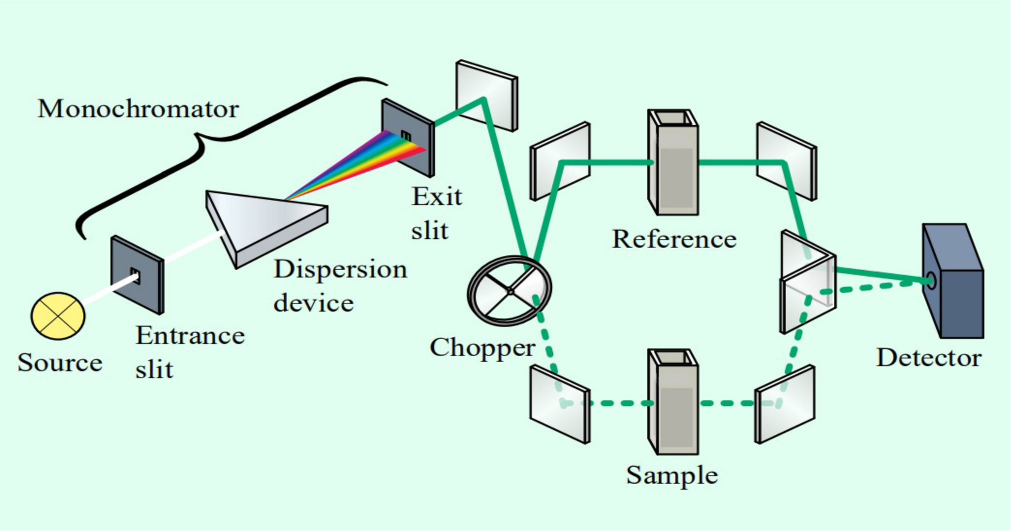

Figure 1: Optical system of a dual-beam spectrophotometer

Uncertainty Analysis

The associated uncertainty must be quoted whenever the results of a measurement are reported. This tells the user of the precision with which the measurement was made. Uncertainty analysis is thus a fundamental part of metrology.

Evaluation of the uncertainty is done by the Guide to the expression of Uncertainty in Measurement (GUM) method. This method is adopted and described in details by International Organization for Standardization (ISO) [12]. The standard uncertainty $u(x_i)$ to be associated with input quantity x_i is the estimated standard deviation of the mean [12, 13].

$$u(x_i) = s(\overline{X}_i) = \left(\frac{1}{n(n-1)}\sum_{k=1}^{n}(X_{i,k} - \overline{X}_i)^2\right)^{1/2}. \qquad (1)$$

The combined standard uncertainty $u_c(y)$ is obtained by combining the individual standard uncertainties u_i, these can be evaluated as Type *A* and Type *B*. That is,

$$u_c^2(y)=\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i). \qquad (2)$$

Expanded uncertainty is calculated according to the following model:

$$U_{EXP}=2U_C=2\sqrt{(U_A)^2+(U_B)^2}, \qquad (3)$$

Where,

U_A: is the uncertainty due the repeatability of the obtained readings; calculated by standard deviation of the mean of repeated five times and,

U_B: is the uncertainty due to standard filters, resolution, drift and stray light. Hence,

$$U_B=\sqrt{(U_{filter})^2+(U_{resolution})^2+(U_{drift})^2+(U_{straylight})^2}, \qquad (4)$$

Where,

U_{filter} = Uncertainty due to reference standard filters at $k = 2$.

U_{drift} = Uncertainty due to drift of the standard, estimated from annual calibrations.

$U_{resolution}$ = Uncertainty due to resolution of the spectrophotometer.

$U_{straylight}$ = Uncertainty due to stray light of the spectrophotometer.

According to the equations model, the calculated accompanied expanded uncertainty with the measurement at k=2 is maximally ± 0.6 % in the photometric (absorbance) scale and ± 0.4 nm in the wavelength scale.

Results and Discussion

In the following illustrations Holmium filter; manufactured in Starna Scientific Ltd [14] is used for calibration of the wavelength scale; was analyzed at bandwidths of 0.1 nm, 0.2 nm, 0.5 nm, 0.8 nm, 1 nm, 2 nm, 3 nm and 5 nm. As you can see from Figures (2, 3), All holmium peaks are clearly appeared especially at high intense peaks 445.7 nm, 453.7 nm and 460.3 at all bandwidths from 0.1 to 3 nm. However, at BW=5 nm the resolution of the device does not able to appear all of them and combined peaks indexed 1,2, see Fig. 4. Hence BW=5 nm is excluded from the Signal-to-noise ratio comparison at Fig.5.

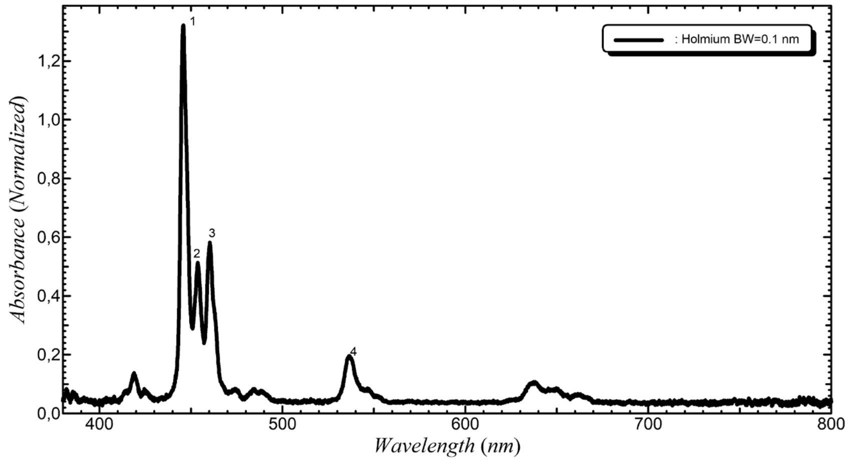

Figure 2: Typical spectrum of a holmium oxide glass filter at BW=0.1 nm

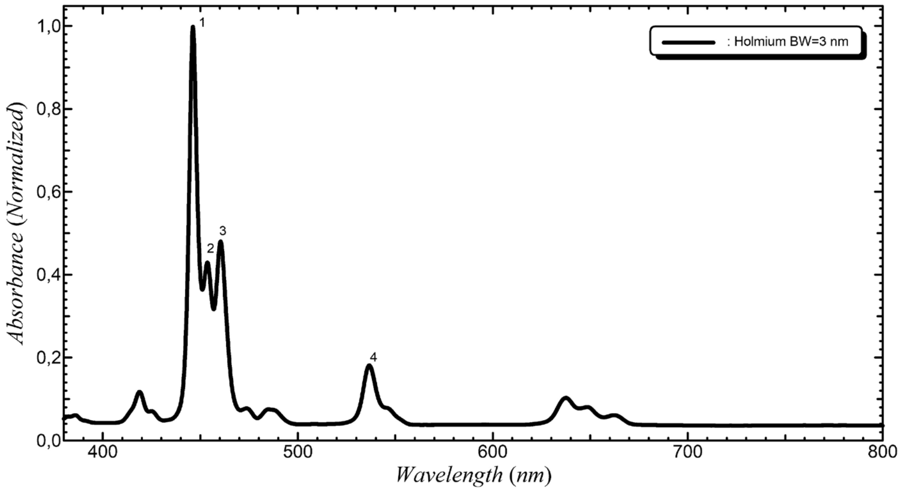

Figure 3:Typical spectrum of a holmium oxide glass filter at BW=3 nm

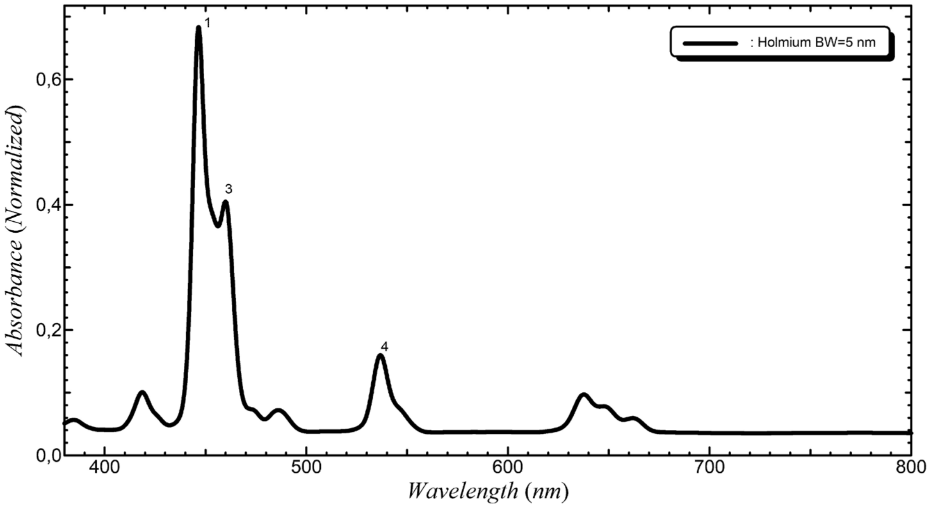

Figure 4:Typical spectrum of a holmium oxide glass filter at BW=5 nm

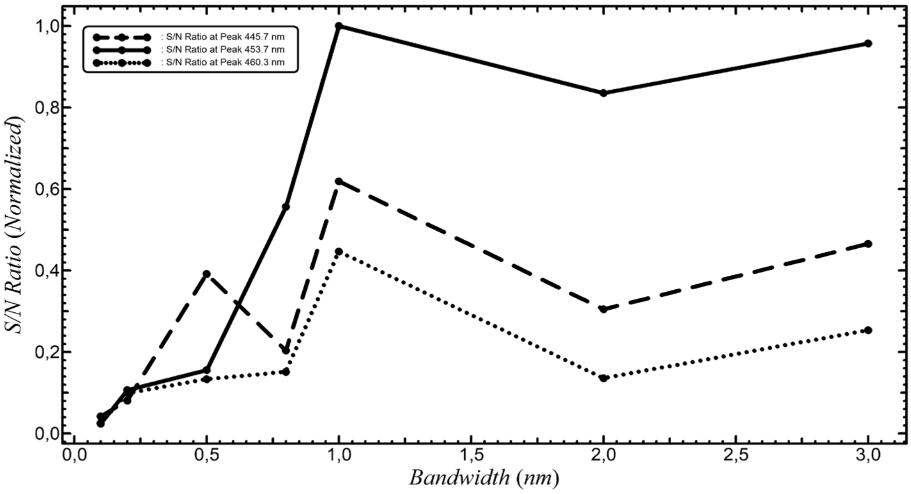

Figure 5: Graphical display of Signal-to-noise ratio vs. spectral bandwidth for Holmium filter at certified peaks 445.7 nm, 453.7 nm and 460.3. The maximum of the plot indicates the maximum S/N occurs at a spectral bandwidth of 1.0 nm.

For our purposes, Noise (N) is defined as the standard deviation σ of a signal's measured values and the signal (S) is the average of those measurements. The Signal-to-noise ratio (S/N) is then the ratio of X to σ.

$$S/N = X/\sigma \qquad (5)$$

The Signal-to-noise ratios of the certified peaks 445.7 nm, 453.7 nm and 460.3 were calculated and the combined information was plotted. According to Fig. 5, the calculated Signal-to-noise ratio of holmium filter is maximized at BW=1 nm. In this case, we can conclude that the analyses of the holmium can be optimized at 1 nm, especially when low limits of quantitation and detection are desired.

Conclusion

The objective of this paper is to obtain the optimum Signal-to-noise ratio accompanied with spectral bandwidths of 0.1 nm, 0.2 nm, 0.5 nm, 0.8 nm, 1 nm, 2 nm, 3nm and 5 nm of peak absorbance of the holmium glass filter. Many 1.0 nm fixed bandwidth instruments are available; however, the optimal bandwidth for an analysis is not necessarily 1.0 nm. According to figure 5, the calculated Signal-to-noise ratio of holmium filter is maximized at BW=1 nm. In this case, we can conclude that the analyses of the holmium can be optimized at 1 nm, especially when low limits of quantitation and detection are desired. Although a narrower spectral bandwidth does improve the resolution of closely spaced peaks, it also decreases the Signal-to-noise ratio. Consequently, a spectral bandwidth should be chosen based on both the needs of the analysis being performed and within the regulatory international guidelines when applicable.

References

1. Biltz, J.P., Klarup, D.G., Signal-to-Noise ratio, signal processing, and spectral information in the instrumental analysis laboratory, *Journal of Chemical Education.,* vol. **79**, p. 1358-1360 (2002).
2. American Society for Testing and Materials (ASTM), Standard Practice for Describing and Measuring Performance of Ultraviolet and Visible Spectrophotometers, ASTM E275 – 08., (2013).
3. American Society for Testing and Materials (ASTM), Standard Practice for Monitoring the Calibration of Ultraviolet-Visible Spectrophotometers whose Spectral Bandwidth does not Exceed 2 nm, ASTM E925 – 09, (2014).
4. Owen., T., Fundamentals of UV-visible spectroscopy, Hewlett-Packard publication., No.12-5965-5123E (2012).
5. Burke, R. W., Mavrodineanu, R., Accuracy in Analytical Spectrophotometry, National Bureau of Standards (NBS). *Special publication.,* 260-81 (1983).
6. C. Decusatis, *Handbook of Applied Photometry Book,* first ed., American Institute of Physics (AIP), (1998).
7. Chan, C. C., Lee, Y. C., Lam, H., and Zhang, X., *Analytical Method Validation and Instrument Performance Verification Book,* first ed., Wiley-Interscience, (2004).
8. Information on http://www.shimadzu.com.
9. Abdelmageed, A., Elmoghazy, E., El-Sharkawy, F., Spectrophotometer Standardization in the UV-Vis Spectral Region*, Journal of Measurement Science and Instrumentation.,* vol.**6**, P. 40-43 (2016).
10. Ashry, Islam; Mao, Yuan; Alias, Mohd Sharizal; Ng, Tien Khee; Hveding, Frode; Arsalan, Muhammad; Ooi, Boon S "Normalized differential method for improving the signal-to-noise ratio of a distributed acoustic sensor" *Applied Optics* **58**(18) 4933-4938, (2019).
11. Riobó, Lucas; Hazan, Yoav; Veiras, Francisco; Garea, María; Sorichetti, Patricio; Rosenthal, Amir "Noise reduction in resonator-based ultrasound sensors by using a CW laser and phase detection", *Optics Letters* **44**(11) 2677-2680, (2019).
12. Guide to the expression of uncertainty in measurement (International Organization for Standardization (ISO), (1993).
13. The expression of uncertainty and confidence in measurement (United Kingdom Accreditation Service (UKAS), Edition-2, (2007).
14. Information on http://www.starna.com/ukhome/d_ref/xrefsets.html.