

A New Approach on the Calculation of Line Width of Gaussian Line Spectra¹

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A new method for the rapid and precise calculation of line width of Gaussian lines spectra is presented. The atomic absorption lines in UV-vis region are Gaussian lines and their line width is given as a function of the ratio of intensity $n = I_0/I_a$ and wavenumber (σ) of the line. The line widths of some pure absorption lines are calculated. The deviation of the calculated values from the measured one is calculated. It is very small in all cases of the observed elements, smaller than 5%.

INTRODUCTION

Spectral analysis means measurements of peak position and of the peak high or peak surface. A powerful technique for separation of overlapped bands is curve fitting method¹, that the measured data should follow a mathematical relationship. Each peak is described by its own function. Lorentzian function^{1,2} or Gaussian function³⁻⁵ mostly describes symmetrical peaks of spectroscopy measurements.

After a mathematical model is chosen on the system under investigation (Lorentzian or Gaussian line shape), the characteristic parameters such as line width, peak position and peak high are calculated¹. The spectral lines in UV-vis region are mainly Gaussian lines³⁻⁵, using mathematical expression (2) to express it. Cameron *et al.*² have used the differential method for precise determination of intensity I_0 and of line width of Lorentzian line shape spectra. They have seen the line width of Lorentzian line shape spectra as a function of the line intensity I_0 and the frequency σ . This paper describes a study of the determination of line width of Gaussian line shape spectra in UV-vis region. It may be noted that the use of a common atomic absorption spectrophotometer, combined with continuous source, is very simple and gives us more precisely and easily calculated results. It is due to the limitation of slit width of the apparatus till 0.1 nm, which causes relatively broad absorption lines⁵⁻⁷. All measurements have been performed in pure standard solutions, free from interference. The method presented might be applied to any Gaussian line spectra, expressed by the following expression:

$$Y_G = A_0 \cdot \exp [-4 \ln 2 / \sigma_D^2 \cdot (\sigma_a - \sigma_0)^2] \quad (1)$$

where A_0 represents maximum absorption intensity centered at σ_0 position, σ_D represents the line width measured at $A_0/2$ position, $\sigma_0 = 1/\lambda$ represents the centre wavenumbers and σ_a represents a wavenumber out of centre wavenumber σ_0 .

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From the mathematical expression (2) of Gaussian line shape spectra we can calculate the intensity of the absorption at any frequency σ_a .

$$A_a = A_0 \cdot \exp [-4 \ln 2 / \sigma_D^2 \cdot (\sigma_0 - \sigma_a)^2] \quad (2)$$

Let us have $A_a = A_0/n$ and $\sigma_D = b$ (3)

Expression (2) should be transformed as:

$$A_0/n = A_0 \cdot \exp [-4 \ln 2 / b^2 \cdot (\sigma_0 - \sigma_a)^2] \quad (4)$$

After transformation of expression (4) we can calculate the line width b as follows:

$$b = 2(\ln 2 / \ln n)^{1/2} |\sigma_0 - \sigma_a| \quad (5)$$

where $n = A_0/A_a$ expresses the ratio of respective absorption intensity in two different positions of frequency or wavelength, σ_0 and σ_a , or λ_0 and λ_a .

Expression (5) gives us the determination of line width b , as a function of intensity ratio (n) and frequency (σ) or wavelength (λ). We can use it for precise calculation of line width of Gaussian line atomic spectra in UV-vis region.

EXPERIMENTAL

Instrumentation: Hitachi-180-80 atomic absorption spectrophotometer (ASS) is used. Some modifications are done in it. Fig. 1 is a schematic diagram of the optical system used in this work. We employed a 250 W halogen lamp as a radiation source. These kinds of lamps are widely used in UV-vis spectrophotometry and was for the the first time used in AAS measurements. Some mirrors and lenses are used to collimate the radiation signal of the lamp. A mechanical chopper is used to pulse the optical signal of the lamp. The measurements are done using 0.1 nm slit width.

LEGEND:

cs	continuous lamp
M ₁ -M ₅	mirrors
L ₁ -L ₅	lenses
S ₁ -S ₃	mechanical slits
CH	chopper
A	atomizer
G	grating
PMT	photomultiplier tube

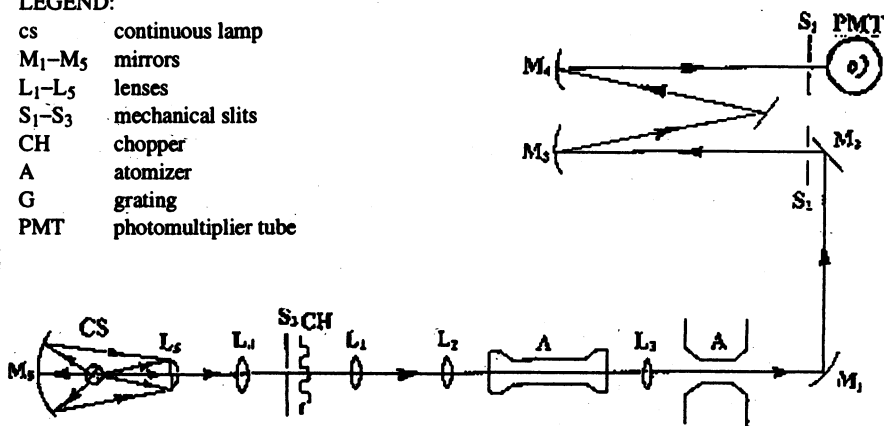


Fig. 1. The schematic diagram of optical system used in Hitachi-180-80 Atomic Absorption Spectrophotometer

Reagents: All the nine standard solutions (Li, Na Cs, Ca, Ba, Sr, Nd, Ho, Eu) were prepared from analytical reagents chemicals and deionized water. The ionization buffer is used.

RESULTS AND DISCUSSION

Continuous source atomic absorption spectroscopy is used for curve fitting and plotting of the nine elements (Li, Na, Cs, Ca, Ba, Sr, Nd, Ho, Eu) in ten different wavelengths, using $I_a = I_0/20$ as base line. We have estimated the line width of the performed lines at $I_0/2$ position, using nm as wavelength unit. The line widths of all obtained absorption spectra were calculated from the expression (5), after the measurements of I_a and σ_a in four different positions ($I_0/10$, $I_0/5$, $I_0/4$ and $I_0/3$). The line width $b = \Sigma b_i/4$ ($i = 1$ to 4) is calculated. The results are listed in Table-1.

TABLE-1
THE LINE WIDTHS OF SOME ABSORPTION LINES

Elements	Element concentration (ppm)	Wavelength (nm)	b_{calc} (nm)	b_{est} (nm)	Relative error (%)
Li*	5.0	570.8	0.055	0.056	2.11
Na*	5.0	589.9	0.050	0.052	3.67
K*	5.0	766.5	0.052	0.051	2.80
Ca*	10.0	422.7	0.051	0.053	3.99
Ba*	20.0	553.3	0.048	0.050	4.26
Sr*	20.0	460.7	0.050	0.052	3.23
Nd†	500.0	491.4	0.046	0.044	4.92
Eu†	20.0	405.4	0.042	0.041	3.45
Ho†	20.0	459.4	0.042	0.040	3.87

*C₂H₂/air flame and 2% CsCl as ionization buffer, in 5% HCl are used.

†C₂H₂/N₂O very reductive flame and 10% LaCl₃ as ionization buffer, in 5% HCl, are used.

Table-1 shows that the absorption lines in UV-vis region are Gaussian lines and the method used for the calculation of their line width is very precise. The relative error between the calculated values b_{calc} and the estimated values b_{est} is very small (rel. error < 5%).

Conclusion

1. After curve fitting of nine absorption lines in visible region, we have found that Gaussian distribution can express their absorption profiles.
2. The method proposed in this paper for the calculation of line width of Gaussian line spectra is very precise. The relative errors between the calculated and estimated values are smaller than 5%.
3. The line width of Gaussian line spectra is given as a function of peak intensity and frequency. It is applicable to any Gaussian line spectra, free from interference.
4. After curve fitting of atomic absorption spectra in UV-vis region, by calculation of spectral line width, we can also use this method to verify the presence of spectral interference in our measurements.

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