Determining Values of Some Optical Constants for Some Colorants

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Received 06 / 12 / 2010 **Accepted** 07 / 03 / 2011

الملخص

تم في هذا البحث إيجاد بعض الثوابت البصرية للعديد من الإصباغ (مواد التلوين) مثل المثيل الأخضر ، المثيل الأحمر ، المثيل البرتقالي ، المثيلين الأزرق، الملكات الأخضر ، البنفسج البلوري ، والسفرانين ومن هذه الثوابت معامل الخمود المولاري ، طول موجة بدء النفاذيه ، طول موجة انتهاء النفاذيه ، معامل التو هين الكتلي ، مساحة مقطع الامتصاص ، طول موجة أقصى امتصاصية (λ_{max}) وعرض نطاق الامتصاص والتي قيمها مهمة في عملية تصنيع المرشحات البصرية. ولقد كانت النتائج على تطابق جيد مع نتائج بعض الشركات المتخصصة في صناعة المرشحات البصرية.

الكلمات الدالة: مرشحات بصرية، أصباغ، معامل الامتصاص.

ABSTRACT

For different dyes like methyl green, methyl orange, methyl red, malachite green, crystal violate, safranin, and methylene blue. We calculated their optical constants like wavelengths of maximum absorption, molar extinction coefficient (molar absorptivity), band width, mass attenuation coefficient, cut on and cut off wavelengths and absorption cross section which are very important in manufacturing the optical filters from these dyes. The calculated results are in good agreement with those values calculated by some specialist companies producing optical filters.

Keywords: Optical filters, Dyes, Absorption coefficient.

INTRODUCTION

The meaning of optical characteristics of a colorants are, molar extinction coefficient, mass attenuation coefficients, spectra of transmittance and spectra of absorbance, wavelength of maximum absorption (λ_{max}), band width, cut on and cut off wavelengths, and absorption cross section. the field concerned with the measurement of these characteristics data is known as spectrophotometry and the instrument employing is called spectrophotometer. the general term colorant components include materials organic and inorganic, that may be used to give color to a substance. this include naturally occurring plant and animal colorants as well as synthetic dyes and pigments.

When we use these colorants to prepare optical filters, we must know some parameters such as: band width (full width at half maximum of absorption or transmission) which used with band pass filter, cut on wavelength(the wavelength at which a filter begins to transmit) which used with long wave pass filter,and cut off wavelength(the wavelength at which a filter ceases to transmit). The cut on and cut off wavelengths specified at 5% of the absolute transmittance point, but band width at ($50\%T_{max}$) (AL- hadedy, 2006).

Dissolve substances have different chemical properties absorb different wavelengths. The optical density of a solution therefore depends on the wavelength of incident light. these dependence is an important factor characterizing of the optical properties of solution. this dependence is expressed graphically as an absorption curve obtain by plotting the wavelength of incident light as the abscissas and the optical density corresponding to these wavelengths as the ordinates.

The mass attenuation coefficient is a measurement of how strongly a chemical species or substance absorbs or scatters light at a given wavelength per unit mass, (hubbell & seltzer, 2007).

Molar mass, **symbol M**, is the mass of one mole of a substance chemical element or chemical compound (international union of pure and applied chemistry, 1993). It is a physical property which is characteristic of each pure substance.

Absorption cross section is a measure for the probability of an absorption process. more generally, the term cross section is used in physics to quantify the probability of a certain particle – particle interaction, e.g., photoabsorption, scattering, etc.

The wavelength of maximum absorption λ_{max} is important for several reasons. the wavelength is characteristic of each compound and provides information on the electronic structure of the analytic. In order to obtain the highest sensitivity and to minimize deviations from Beer's law, analytical measurement are made using light with a wavelength of λ_{max}.

THEORY

When electromagnetic radiation passes through homogeneous isotropic material, its intensity reduced. bougers law, also called Lambert's law or, Lambert –bouguer law, relates to the transmittance of an absorbing materials to its thickness x (Driscoll and Vaughan, 1978).

$$T = e^{-kx}$$

The spectral absorption coefficient (k) depends on the nature of the absorber and is a function of the incident wavelength (Sybil, 1988).

Beer draw attention to the similar law for homogeneous materials (in particular liquids and some gasses), for variation the concentration of the absorbing component rather than for variation in thickness, Beer's law states that the transmittance of a liquid absorber is given by the following equation:

$$T = e^{-\beta C X}$$

$$\log T = - \beta c\ x / 2.303$$

$$\log T = \epsilon\ c\ x$$

The value of (ϵ) in above equation depends on the unit of concentration (c), if the concentration of the solute is expressed in moles per liter, the constant is called the molar extinction coefficient or molar absorptivity, its value of the absorption solute usually changes with the wavelength of radiation, with temperature of the solution and with the solvent (Sybil, 1988).

The dimensionless product in above equation is called optical density or absorbance (A) (Tilley, 2000), then can be written.

$$A = \epsilon\ c\ x$$

When there is more than one absorbing species in a solution, the overall absorbance is the sum of the absorbance for each individual species (x, y etc.) (Lakowicz and Goseph 2006)

$$A = (\epsilon_x c_x + \epsilon_y c_y + \ldots\ldots) x$$

Plots of the quantities, T and A as a function of wavelength λ are called specerophotpmetric curves. from these curves cut on and cut off wavelengths, wavelength of maximum absorption (λ_{max}) and band width of absorption can be calculated (kirk – othmer, 1966).

The Plot of A as a function of concentration measured in cell of constant thickness (1 cm), yield straight line, the slope of which is equal to the molar absorptivity (Sybil, 1987).

$$\epsilon = A \;/\; c\,x$$
$$x = 1\text{cm}$$
$$\epsilon = \text{slope}$$

The molar absorptivity (ϵ) is directly related to the absorption cross section (σ) via the Avogadro constant (N) in units cm^2 (lakowicz & joseph, 2006).

$$\sigma = 2303\ \epsilon \backslash N = 3.82 \times 10^{-21}\ \epsilon$$

The molar absorptivity is also closely related to the mass attenuation coefficient, as shown by the equation
(mass attenuation coefficient) (molar mass) = molar absorptivity

The molar mass of a compound is given by the sum of the standard atomic weights of the atoms which form the compound multiplied by the molar mass constant, M_u =1 g / mol : (Mohr & Taylor, 2005).

EXPERIMENTAL

Specific weight of colorant dissolved in specific volume of distilled water, then stirred by magnetic hot plate stirrer to get homogeneous aqueous solution. Colorant solution was placed in a glass vessel with parallel wall (a cell), its thickness 1 cm then measuring the absorbance (A) and transmittance (T) for the range (400 – 700) nm by employing spectrophotometer device type shemadzu uv –visible– 160 A. The values of A and T were plotted as a function of wavelengths from which we get λ_{max}, band width and cut on and cut of wavelengths.

Six different concentrations of each colorant were prepared by dulation method and then measuring the absorbance of each colorant at λ_{max} we had been found. The relation between concentration and absorption was plotted, then fitting the straight line. The slope of each line represent the molar absorptivity and also the mass attenuation coefficient and absorption cross section were calculated.

RESULTS and DISCUSSIONS

Fig (1) shows the transmittance of seven colorants. We can see the range of wavelengths at which the materials have high transmittance and the range of wavelengths at which the transmittance nearly zero.

These results can offer us the ability to manufacture a proper filters, like short wave pass filter from methylene blue dye, band pass filter from methyl green, malachite green, and crystal violate dyes, long wave pass filter from methyl red, safranin and methyl orange. Also from this figure we show that the spectrums of methyl red and safranin have small difference between them but they differ from methyl orange which give very good long wave pass filter, since it absorb blue wavelength greeter them. There is a similarity between malachite green and methyl green. The methylene blue could be good short wave pass filter because it absorbs red wavelengths.

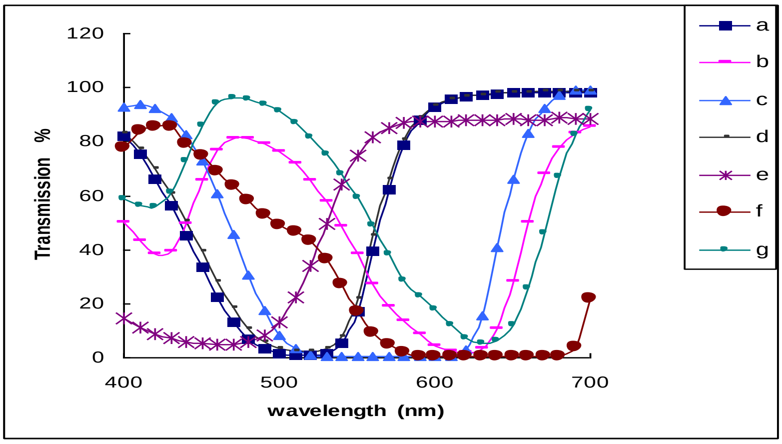

Fig.1: Visible transmission spectra of the colorants:a-safranin,b-malachite green, c- crystal violet, d- methyl red, e-methyl orange, f-methylene blue and g- methyl green.

Figure (2) represent the spectral absorbance of the colorants from which λ_{max} and band width of absorption can be found. These spectrums show how the absorbance of light for colorant depends upon the wavelengths of the incident light. From this figure we show that methyl green and malachite green absorb blue, yellow, and orange wavelengths. Methylene blue absorb red light. Crystal violet absorb green and yellow but transmit blue and red light.

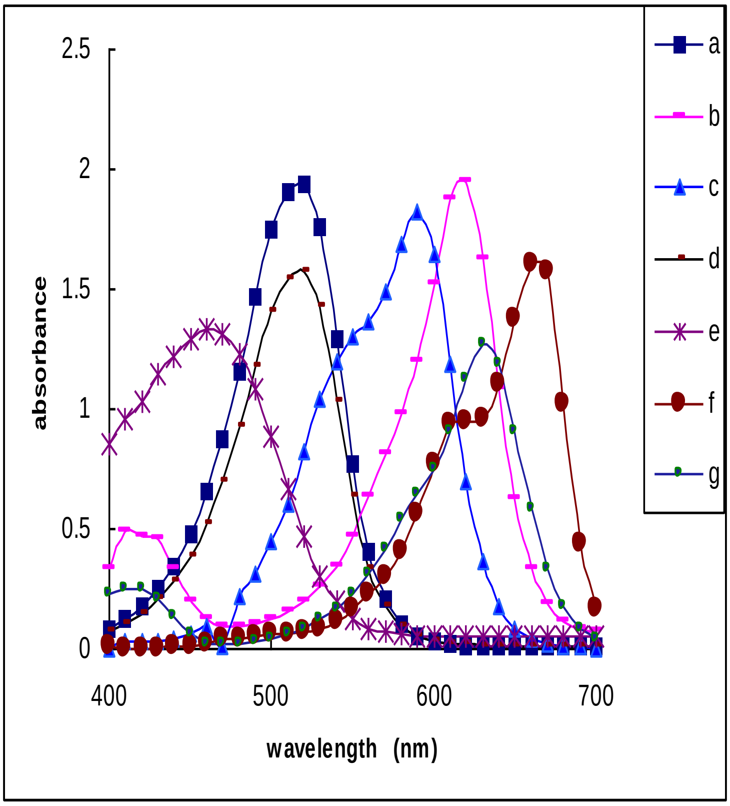

Fig.2: Visible absorbance spectra of the colorants :a-safranin, b-malachite green, c- crystal violet, d- methyl red, e-methyl orange, f-methylene blue and g- methyl green.

The absorbance (A) as a function of concentration for each colorant are shown in figures 3(a-g). It can be noted that the relations are straight line, which agreement with Beer's law. The slope of each one represent molar extinction coefficient. Also this figure represent calibration curves that relates the concentration of each dye with its absorbance at its wavelength of maximum absorption.

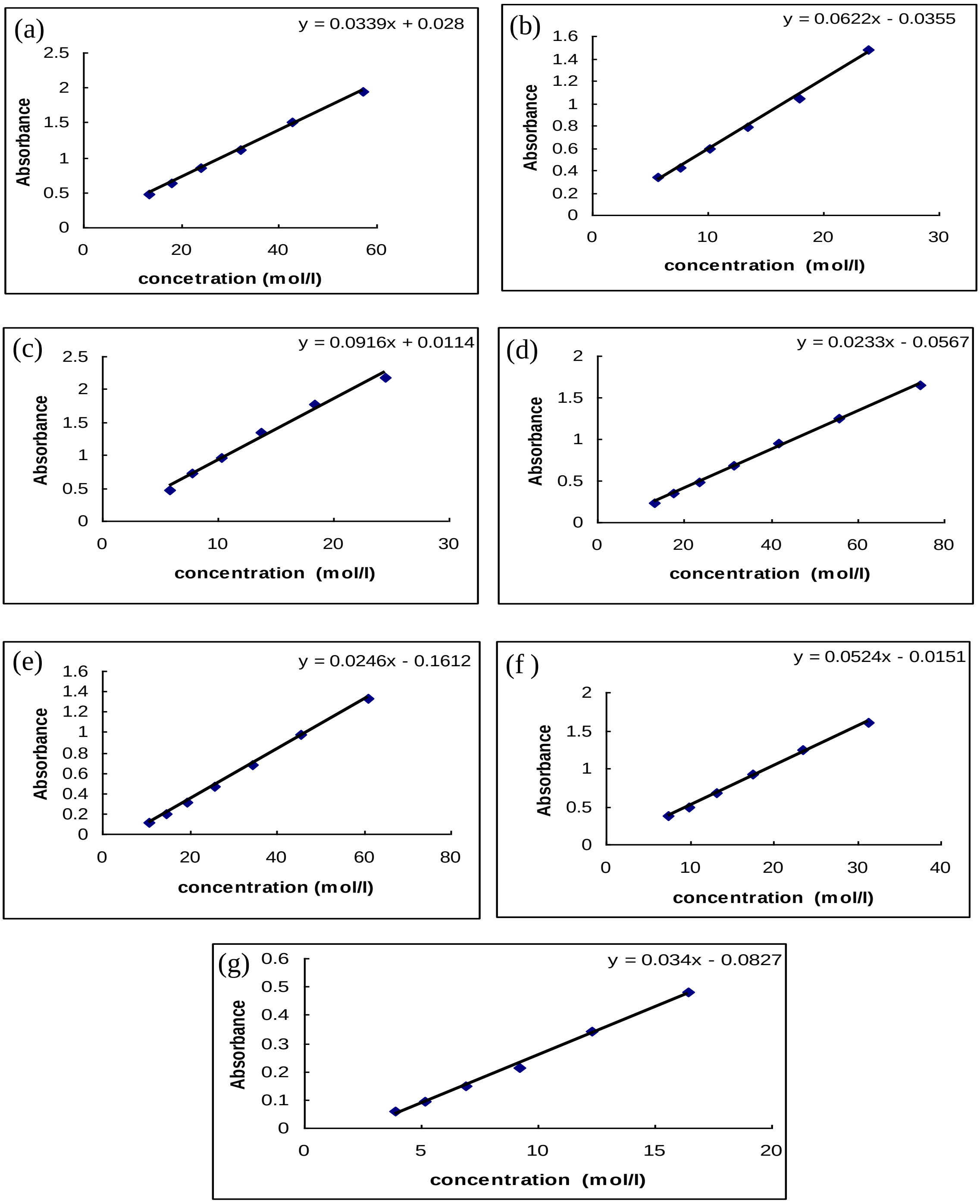

Fig.3: Absorption as a function of concentration of the colorants: a-Safronin, b-malachite green,- crystal violet,d- methyl red,e-methyl orange, f-methylene blue and g- methyl green.

Table(1) show the constants: wavelength of maximum absorbance (λ_{max}), molar extinction coefficient (ϵ_{λ}), cuton and cutoff wavelengths, mass attenuation coefficient, absorption cross section and band width that we found for each colorant. Also we see that the cool dyes (crystal violet, and methylene blue) have attenuation to the light greater than hot dyes (methyl red, methyl orange, and safranin).

Table (1) : Spectral properties of the colorants materials of maximum absorption.

Colorant	λ_{max} (nm)	Molar Extinction Coefficient (L/ mol.cm)	Cuton wavelength (nm)	Cutoff wavelength (nm)	Mass attenuation coefficient (L/cm. g)	Absorption Cross section $x10^{-21}$ (cm^2)	Band width (nm)
Methylene blue	665	52400		568	377.281	200168	602-683
Methyl green	631	34000			128.621	129880	590-658
Malachite Green	616	62200			342.204	237604	580-642
Crystal Violet	590	91600			857.648	349912	525-615
Safronin	518	33900	541		222.521	129498	475-546
Methyl red	515	23300	536		199.249	89006	474-547
Methyl orange	462	24600	465		173.073	93972	-508

Table 2 show how λ_{max} differ from company to others and some time the company itself give different value of λ_{max}

Table (2): Comparison between the wavelength of maximum absorption of our research with other publisher companies. Aldrich chemical catalogue (1992), Lillie (Conn's Biological Stains), Edward Gurr (1971),

colorant	λ_{max} / nm Our Research	λ_{max} /nm Aldrich	λ_{max} / nm Conn	λ_{max} /nm Gurr
Crystal Violet	590	588		593
Methyl Green	631	657	630 – 634, 420	
Methylene Blue	665	661	664 - 666	665
Methyl Orange	462	505, 507		
Methyl Red	515	493,437,410		
Safranin	518	530		
Malachite Green	616	614, 425	617- 619, 425	618

CONCLUSION

From this study we obtain the constants, molar extinction coefficient wavelength of maximum, absorption, cut on and cut off wavelengths, mass attenuation coefficient, absorption cross section, and band width for some colorants which are used for manufacturing a proper optical filters, and these results are in good agreement with some reference and differs from others. Also we conclude that wavelength of maximum absorption must calculated experimentally since its value differ for different companies also differ for one company.

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