Linear Optical Properties of Nile BlueDye Dissolved in Different Solvents

Rajaa K. Khleif[1], Talib M. Abbas [2]

[1,2]Department of Physics, College of Education for Pure Sciences, University of Babylon,Babylon, Iraq.

Abstract:

In the presentwork, the optical properties and absorption spectrumof laser Nile blue dye(NB) dissolved in different solvents (distilled water, ethanol, methanol) at different concentrations were studied.The results showed that increasing the concentrations leads to an increase in the absorbance and a decrease in transmittance for the prepared sample, and thus an increase in the linear optical properties (linear absorption and refraction coefficients, respectively).When comparing the three solvents and their impact on the absorption of thedye, noted that the absorbance values for methanol are much greater it is in ethanol and water. These differences are due to the different properties of the solvent in terms of polarity and hydrogen bonding ability.

Keywords : Solvents, Nile Blue Dye, linear optical properties
DOI Number: 10.14704/nq.2022.20.5.NQ22571 **NeuroQuantology 2022; 20(5):2072-2082**

1 Introduction

In the visible range of the electromagnetic spectrum, organic dyes have a significant absorption band. Only organic molecules with an extended system of conjugated bonds alternating single and double bonds have this feature. The shift from the electronic to the absorption bond ground state S0 to the first excited singlet state S1 is attributable to dyes' long-wavelength absorption band. This process is often quite significant, giving rise to an absorption bond ground state S0. With oscillator strength on the order of unity, the transition moment occurs. The spontaneous emission in dye lasers is caused by the reversal process S1 to S0.(Duarte & Hillman, 1990).It had been Dye lasers are used for sensing jobs, analytical chemistry, and other measurements, and are one of the most significant and commonly utilized applications in many areas of life. Liquid dye lasers can provide the ability to tune light sources.

Liquid dye lasers have a very wide fluorescence optical band and are commonly used in the visible wavelength region as tunable narrow bandwidth light sources 400 nm to 900 nm. There are a variety of laser dyes available, all of which are quite efficient. One of these dyes, Nile Blue, has a wide range of uses in biology, chemistry, and physics(Azzouz et al., 2006).

2.The Theoretical Part

2.1. Linear optical properties:

The optical properties of materials are generated when incident light interacts with the material (Klinowski, 2005) by absorbing the light in the medium. The other part is called the penetrating radiation, as it passes inside the material without losing energy, and the other part is reflected from the surface of the sample (Fowles, 1989), and in some samples part of the scattered light. To study the properties of the internal synthetic material, the properties of absorption, reflection, and penetration of the material must be studied. For example, the structure of energy levels and transition possibilities are discovered through the study of ultraviolet spectra, and the study of the visible spectra of the material is also used to employ the material in various applications(Jannson, 2005).

1.Absorbance:

The process by which radiation transfers some or all of its energy to the material through which it passes meaning is The process of decreasing the intensity of certain frequencies (certain wavelengths) of electromagnetic radiation results in Electrons rising from a certain level to a higher energy level due to the interaction between a binary moment. The electrode of these particles and the electric component of electromagnetic radiation (photon). In the case of liquid materials, the potential of a solution to absorb incident photons is directly proportional to the concentration of the absorbed particles in the sample. The mathematical expression between the density of particles (concentration) in the sample, as well as the sample's thickness Through which the incident ray passes the optical path length,is the absorbance or optical density(Andreasen et al., 2011):

$$A = Iog_{10}\left(\frac{I_{\circ}}{I}\right) = \varepsilon \ell C$$

Where that:
I: is the intensity of photons flowing through the sample at the wavelength (transmitted intensity).
I_o: is the intensity of the incident rays before they enter the sample.
C: sorbent concentration.
ε: molar inertia coefficient and its units($cm^{-1}M^{-1}$).
ℓ: the thickness of the material through which the incident ray is passing.

The material absorption of the incident ray will cause an electronic transition if the energy value of The substance absorbed by the substance is sufficient to move to a higher energy level, and Beer Lambert's law states that the probability of The absorption of incident photons by matter increases with increasing concentration of matter (Fowles, 1989).

[Beer.'s law] Lambert There is an empirical relationship between the absorption of photons andthe qualities of the material through which the rays flow.The law states that the amount of light absorbed is proportional to the number of particles. that absorb it When radiation enters a solution, the amount of radiation absorbed or transmitted is an exponential function of the solution's concentration.(Solute) (Li et al., 2008),(Fowles, 1989).

Therefore, if the radiation used is Light Monochromatic. Beer Lambert's law can be applied to a variety of spectral regions, including UV radiation, visible light, and so on(Verhaegen & Drowart, 1962).

2.Transmittance (T):

The permeability to the middle (T) is the ratio of the transmitting intensity (I) to the incident intensity (I_0) after The medium absorbs part of the incident ray, so the transmitted ray is the result of an incident ray that has undergone absorption inside The material passing through it or it is the radiation flowing from the medium to the radiation falling on it i.e.(Parikh, 1974)(Demtröder, 2010)

$$\mathrm{T} = \left(\frac{I}{I_{\circ}}\right)$$

According to Beer-Lampert's law, the permeability decreases with increasing molar concentration (c) and Optical path length (ℓ) through which light passes (McWeeny, 2007)

$$T = \frac{I}{I_\circ} = 10^{-\varepsilon c \ell}$$

Where the absorbance of the medium is related to the permeability, the incident intensity and the penetrating intensity in the following relationship (Menzel, 2013)

$$A = log_{10}\left(\frac{I_\circ}{I}\right) = -log_{10}(T)$$

From this relationship noted that the transmittance (T) depends on the medium's absorption, the higher the absorbance The lower the average permeability.

2.2.Optical Parameters

1.Absorption coefficient:

The absorption coefficient (α_o) or the attenuation of the intensity of light passing through a substance i.e. a factor expressed as Part of the absorbed beam for a unit thickness of Article (Nelson, 2003)According to Beer-Albert's law. the coefficient of Absorption can be found through the following relationship (Straughan & Walker, 1976):

$$2.303A = \alpha_\circ \ell$$

$$\alpha_\circ(cm^{-1}) = 2.303\ \frac{A}{\ell}$$

$$\alpha_\circ = \frac{1}{d} ln(\frac{1}{T})$$

Where: (A) represents absorption, (T)Transmittance

2.Refractive index (n):

The refractive index is an essential parameter for any optical material, usually Maxwell's wave equations Primary source for deriving important visual properties, definitions, formulas, and basic concepts for materials. For a transparent optical material, the refractive index (n) is simply defined as the velocity ratio (c) of an electromagnetic wave in a vacuum to the phase velocity (ν) of the same wave in material (Jackson, 1962) i.e.:

$$n = \frac{c}{\nu}$$

The refractive index isn't constant but rather depends on the electromagnetic wave's length falling on a substance-specific Alsoexceptfor some materials. the refractive index also varies depending on the direction of thewaves The substance is electromagnetic, and these materials are utilized to change the polarization direction of this wave(Hollas, 2004). so Complex refractive index can be determined:

$$\bar{n} = n + ik$$

*e*ISSN 1303-5150

where k is the damping coefficient or absorption coefficient (or the imaginary part of a complex refractive index). Both (k and n) depend on the frequency of the wavelength. The damping coefficient K can be calculated from the equation following (Brown & Arnold, 2010):

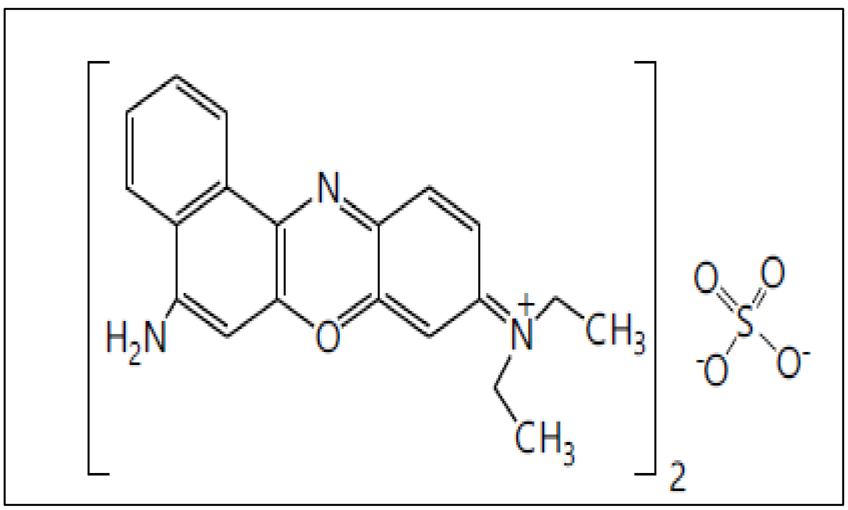
$$\kappa = \frac{\alpha_o \lambda}{4\pi}$$

The refractive index indicates the degree to which a material is affected by electromagnetic waves, so when the radiation falls Electromagnetic conduction on the material works to move the charge in the material from its original position which results in a dipole, so if (υ) is the frequency of the alternating electric field of the electromagnetic wave Thus, the electrical polarization of the molecule will oscillate at the same frequency (υ), so it will beConverting a portion of the incident wave energy into the created electrode dipole's vibrationenergy and thus Reduce the incident wave amplitude Assuming that the energy loss causes thedipole to oscillate slightly (László, 2003),So it is obvious that the material's polarization is caused by electromagnetic fields, radiationfalling on the material has A refractive index measurement of a substance, so the higher thepolarization, the greater the effect of the delay, and the higher the refractive index

The speed of light in the material decreased, and the material that does not have polarization does not have any delay in returning the lightTherefore, its refractive index (1=n)(Davies, 1963).

3.Experimental Part
3.1. Materials Used
1. Nile Blue Dye

Nile blue dye is classified as a phenoxazine dye(Sabnis, 2010).Nile Blue dye has a positively charged, oxidized, phenoxazine system, the high fluorescence and intensity of Nile Blue dye are good indicators of the polarity of the dye's circumference.Nile Blue dye exhibited progressively high absorption and emission as the solvent polarity is increased. The spectroscopic characteristics of Nile Blue dyeare pH-dependent(Jose & Burgess, 2006). Figure (1),shows its molecular structure. It's chemical formula is ($C_{40}H_{40}N_6O_6S$) with molecular weight Mw=: 732.85 gm/mol (Sabnis, 2010).



Figure(1): Molecular structure of Nile Blue dye(Sabnis, 2010).

2.Solvents:

In the present work,three organic solvents have been used Ethanol (Ethyl Alcohol) whose molecular formula is C_2H_5OH and molecular weight of46.04 gm /mol, methanol solvent (Methyl Alcohol) with its molecular CH_3OH and the molecular weight is 32.04 gm/molfrom (Spain country) with a purity of 99.9%, and distilled water solvent (H_2O).

4.Solutions preparation:

The Nile blue solutions used in the current study were prepared by dissolving the dye powder (0.018) gm in a volume (30) ml solvent ethanol where the concentration was obtained (1×10^{-3}) M according to the following equation :(Saito et al., 1990)

$$W = \frac{V \times C \times Mw}{1000}$$

Where W: weight of the dissolved in material (g), $M_{W:}$ Molecular weight of the material (gm/ mole), V:volume of the solvent (ml), and C: the concentration (M).

The prepared solutions were diluted according to the following equation: -

$C_1 V_1 = C_2 V_2$

Where

C_1: primary concentration

C_2: new concentration

V_1: the volume before dilution

V_2: the volume after dilution

Three concentrations were prepared (0.1,0.3and 0.5mM) respectively as shown in Figure (2-a,b,c)

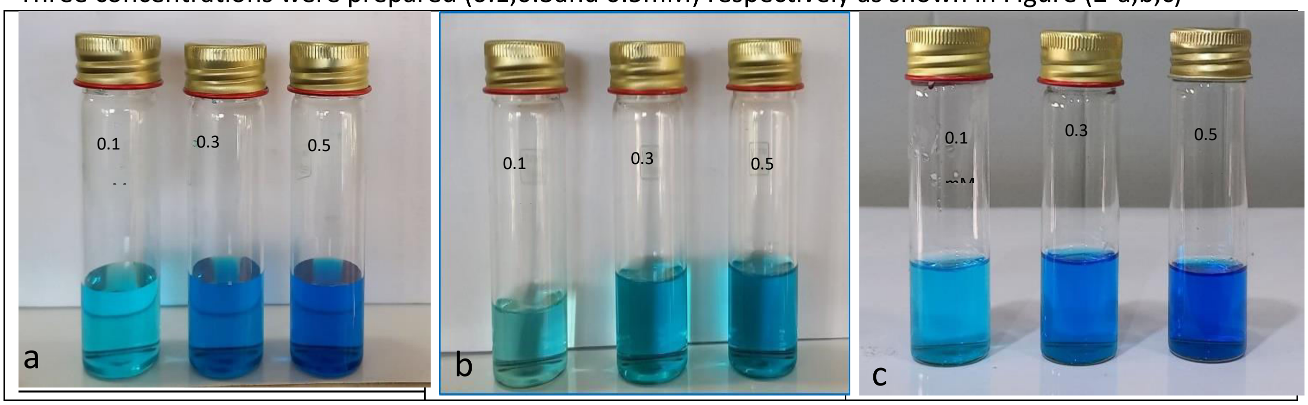
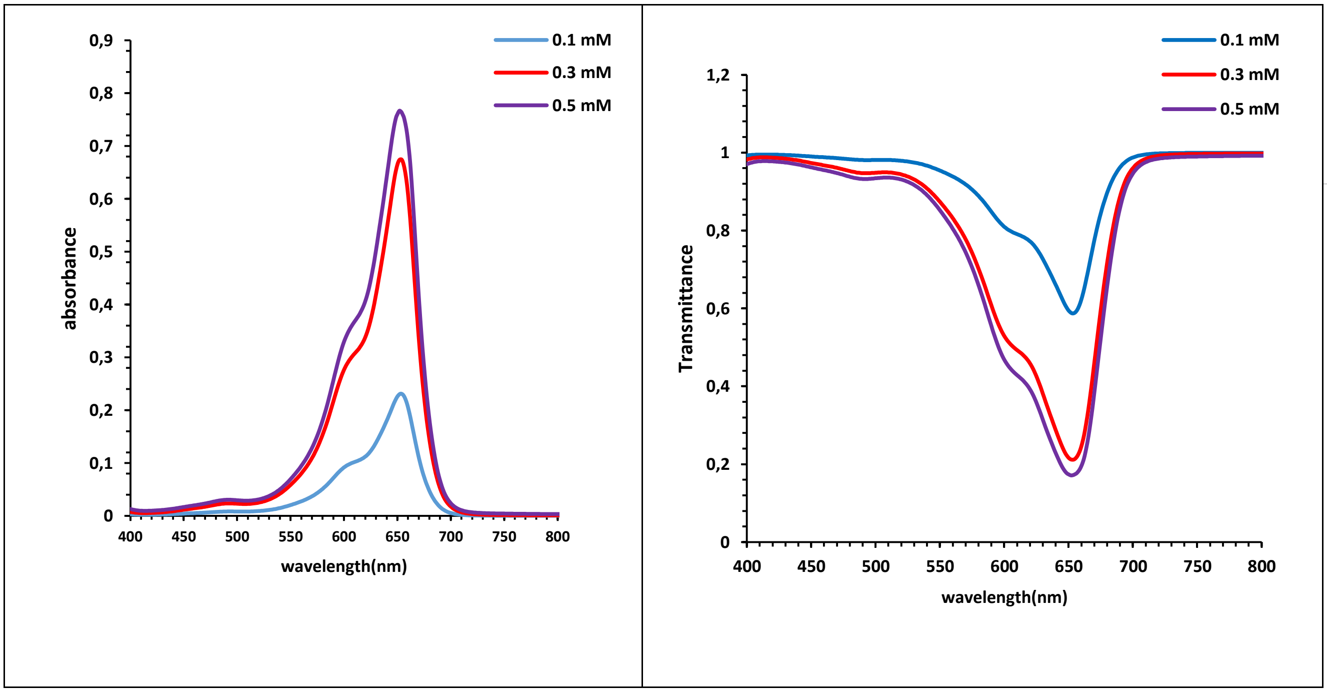


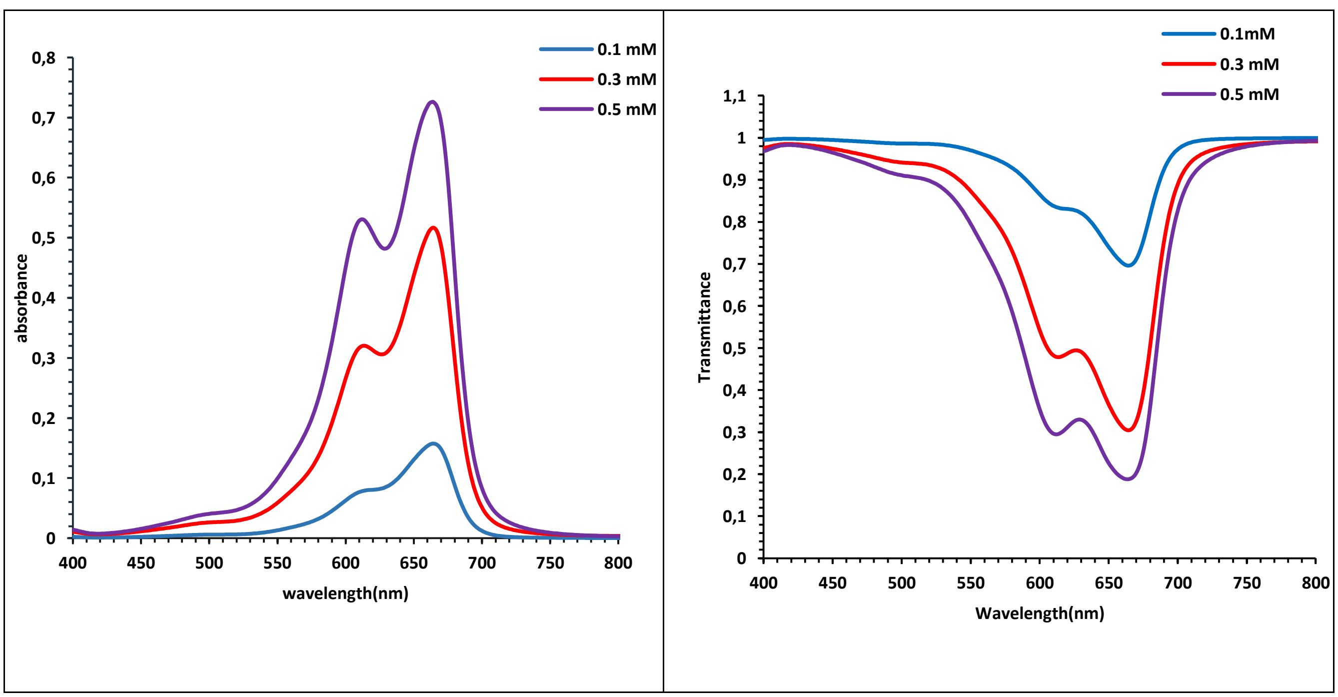
Figure (2): The solutions samples ofNB dye at different concentrations in a. water solvent. b. ethanol solvent. c. methanol solvent.

5.Results and Discussion:

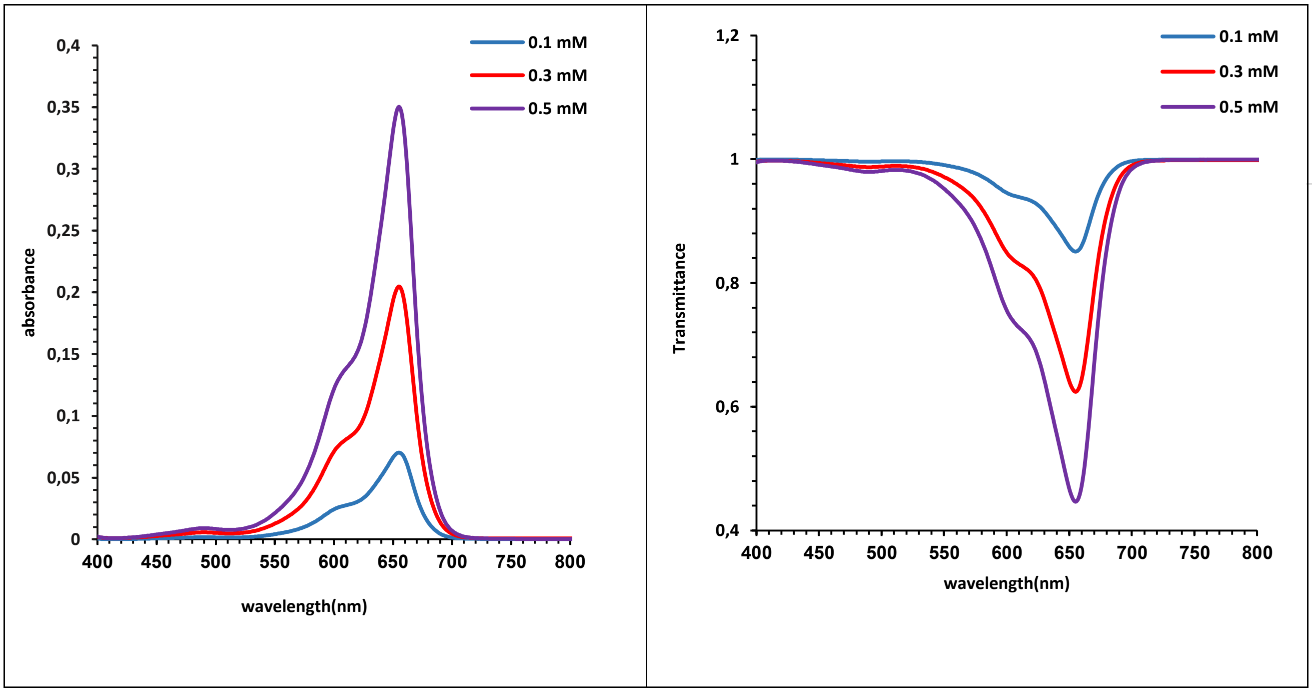
The figure shows 3(a,b,c)the absorption spectrum of Nile blue dye solutions dissolved in solvents (methanol,distilled water, and, ethanol) at different concentrations (1×10^{-5}M, 3×10^{-5} M, 5×10^{-5} M) and it is noted that the increase in concentration leads to an increase in the absorbance and decrease transmittance accordingtoBeer- Lambert's lawin this case.


0.1 mM
0.3 mM
0.5 mM
absorbance
wavelength(nm)
Transmittance
wavelength(nm)

(a)


0.1 mM
0.3 mM
0.5 mM
absorbance
wavelength(nm)
0.1mM
0.3 mM
0.5 mM
Transmittance
Wavelength(nm)

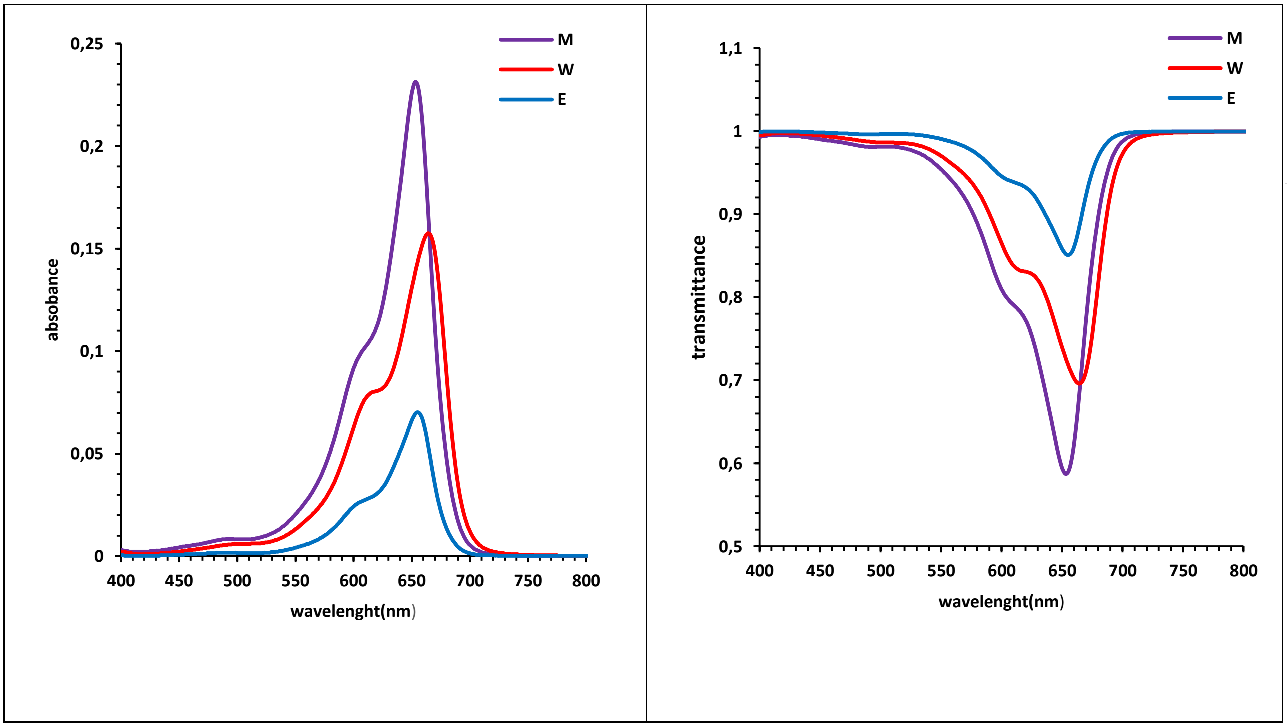
(b)



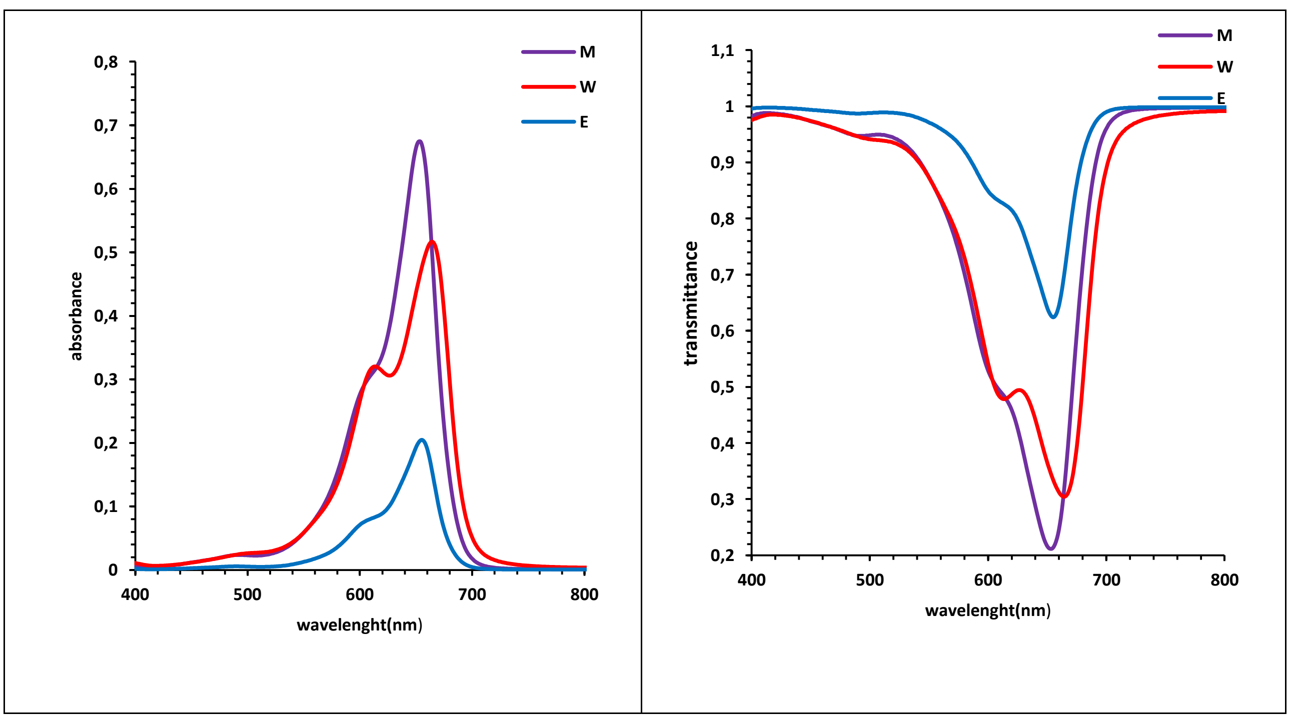
(c)

Fig (3): The Absorbance and transmittance spectraof NB dye solutions at different concentrationsin a- methanol solvent b- water solvent c- ethanolsolvent

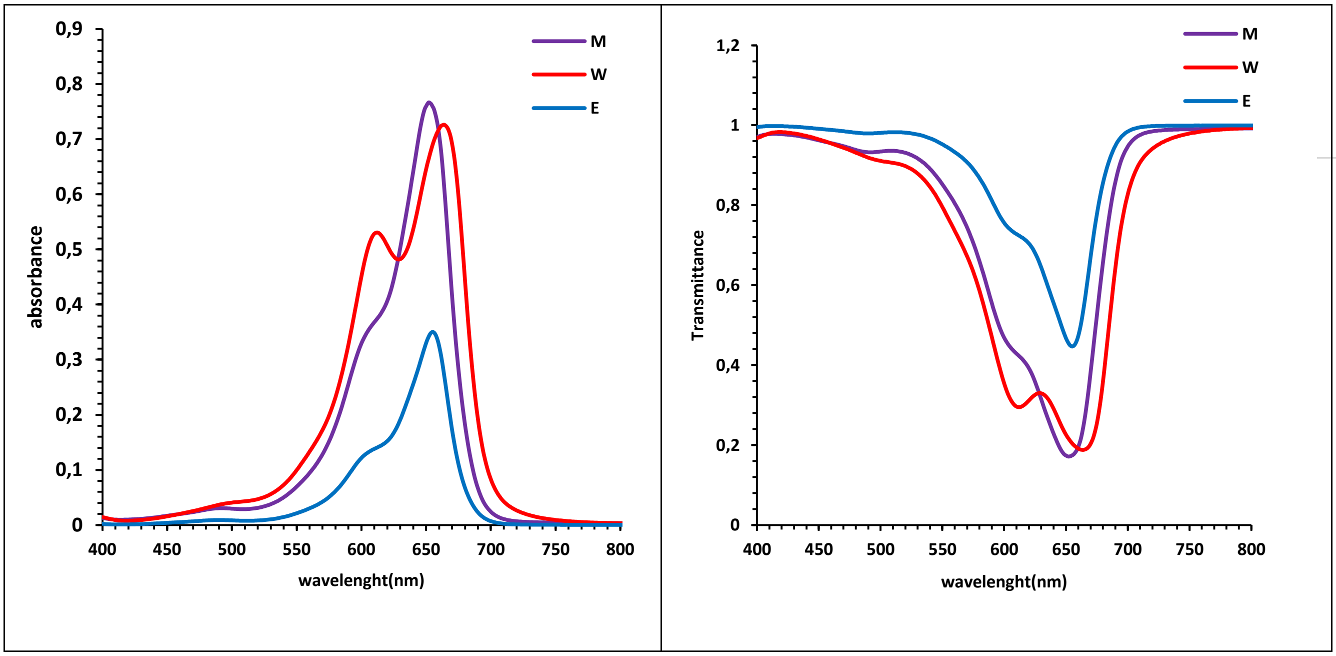
Figures (4)a,b, and c show the absorption and transmittance spectra of concentrations(1×10^{-5},3×10^{-5},5×10^{-5}) M in the solvents (methanol, distilled water, ethanol).It was found that Nile blue dye has good solubility in water and gives two absorption peaks at the wavelength(613 to 664)nm and that the maximum absorption value changes from(613-664) nm with increasing concentration, but when the dye is dissolved in absolute methanol, the absorption spectrum gives one peak at the wavelength (653)nm with increasing absorption, while when dissolving the dye in ethanol It gives one peak at wavelength (655) nm, so methanol was adopted as a solvent for the dye in this study.


M
W
E
0,25
0,2
0,15
0,1
0,05
0
absobance
400 450 500 550 600 650 700 750 800
wavelenght(nm)
1,1
1
0,9
0,8
0,7
0,6
0,5
transmittance

(a)


M
W
E
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
absobance
400 500 600 700 800
wavelenght(nm)
1,1
1
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
transmittance

(b)



(C)

Fig (4): The Absorbance and transmittance spectra ofNB dye solutions in a different solventatconcentrations a.(1×10^{-5} M)b.(3×10^{-5} M)c- (5×10^{-5} M)

Table (1) shows the values of absorbance, transmittance, linear absorption coefficient, and linear refractive index, where we notice an increase in the linear absorption coefficient and the linear refractive index, and that the reason for increasing the linear refractive index depends on the density of the solution, meaning that the higher its density, the higher the absorption coefficient.

Table (5) The linear optical properties of NBdye dissolved in a different medium

Solvents	C(M)	λ(max)	A	T	$\alpha(cm)^{-1}$	n_o
Methanol	1×10^{-5}	653	0.23	0.58	0.53	1.27
	3×10^{-5}	653	0.67	0.21	1.55	1.55
	5×10^{-5}	653	0.76	0.17	1.76	1.99
Disitlled Water	1×10^{-5}	664	0.15	0.69	0.36	1.75
	3×10^{-5}	664	0.51	0.30	1.18	1.98
	5×10^{-5}	664	0.72	0.18	1.67	2.39
Ethanol	1×10^{-5}	655	0.07	0.85	0.16	1.36
	3×10^{-5}	655	0.20	0.62	0.47	1.91

	5×10^{-5}	**655**	**0.35**	**0.44**	**0.80**	**2.15**

6. Conclusions:

Increasing the concentration of the dye will lead to an increase in the absorbance, and Beer-Lambert's law is in agreement with this., and thus increase the linear optical coefficients refractive index and absorption coefficient) for all prepared samples. Linear optical properties, especially the locations and width of the absorption spectra, depend on the type of solvent, as it affects the probability of electronic transitions. Therefore, it is noted that there are two peaks of the absorption spectrum of the dye dissolved in water in the visible light region, and the reason for this is that the polarity of water is much higher than that of ethanol, and also the possibility of water on the affinity of its molecules and the formation of hydrogen bonds that allow more bonds with the dye molecules, which can lead to a change in the order of energy levels of the dye molecule.

References:

Andreasen, J., Sebbah, P., & Vanneste, C. (2011). Nonlinear effects in random lasers. *JOSA B*, *28*(12), 2947–2955.

Azzouz, H., Alkhafadiji, L., Balslev, S., Johansson, J., Mortensen, N. A., Nilsson, S., & Kristensen, A. (2006). Levitated droplet dye laser. *Optics Express*, *14*(10), 4374–4379.

Brown, M. S., & Arnold, C. B. (2010). Fundamentals of laser-material interaction and application to multiscale surface modification. In *Laser precision microfabrication* (pp. 91–120). Springer.

Davies, M. (1963). *Infra-red spectroscopy and molecular structure*.

Demtröder, W. (2010). *Atoms, molecules and photons* (Vol. 3, Issue 7). Springer.

Duarte, F. J., & Hillman, L. W. (1990). *Dye laser principles, with applications*.

Fowles, G. R. (1989). *Introduction to modern optics*. Courier Corporation.

Hollas, J. M. (2004). *Modern spectroscopy*. John Wiley & Sons.

Jackson, J. D. (1962). : *Classical electrodynamics. John Wiley and Sons, Inc., New York-London-Sydney, 641 p*.

Jannson, T. P. (2005). *Tribute to Emil Wolf: Science and engineering legacy of physical optics* (Vol. 139). SPIE Press.

Jose, J., & Burgess, K. (2006). Benzophenoxazine-based fluorescent dyes for labeling biomolecules. *Tetrahedron*, *62*(48), 11021–11037.

Klinowski, J. (2005). High-Resolution Molecular Spectroscopy Electronic Spectroscopy. *University of Cambridge*.

László, P. (2003). *A LiNbO3 nemlineáris optikai tulajdonságainak vizsgálata Z-scan módszerrel*. Ph. D. thesis, Szegedi Tudományegyetem.

Li, J., Wang, M., Lin, Z., Huo, X., & Zhai, G. (2008). Optical linearity and nonlinearity of ZnSe nanocrystals embedded in epoxy resin matrix investigated by Z-scan technique. *Ceramics International*, *34*(4), 1073–1076.

McWeeny, R. (2007). *Atoms, molecules, matter–the stuff of chemistry*. Italy.

Menzel, R. (2013). *Photonics: linear and nonlinear interactions of laser light and matter*. Springer Science & Business Media.

Nelson, J. A. (2003). *The physics of solar cells*. World Scientific Publishing Company.

***e*ISSN** 1303-5150

Parikh, V. M. (1974). *Absorption spectroscopy of organic molecules*. Reading, Mass.: Addison-Wesley Publishing Company.

Sabnis, R. W. (2010). *Handbook of biological dyes and stains: synthesis and industrial applications*. John Wiley & Sons.

Saito, Y., Kato, M., Nomura, A., & Kano, T. (1990). Simultaneous three primary color laser emissions from dye mixtures. *Applied Physics Letters*, *56*(9), 811–813.

Straughan, B. P., & Walker, S. (1976). Molecular Quantum Numbers of Diatomic Molecules. In *Spectroscopy* (pp. 1–25). Springer.

Verhaegen, G., & Drowart, J. (1962). Mass Spectrometric Determination of the Heat of Sublimation of Boron and of the Dissociation Energy of B2. *The Journal of Chemical Physics*, *37*(6), 1367–1368.

***e*ISSN** 1303-5150