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Study of the Effect of Concentration on the Absorption Spectrum of Copper-Phthalocyanine Dye (CuPc)

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ABSTRACT

This present Work was undertaken to study some the photo physics properties of copper-phthalocyanine dye (CuPc), in solvent Dioxane separately under normal circumstances at (room temperature) in different concentrations (1×10^{-3} , 1×10^{-4} , 0.5×10^{-4}) m / l. The intensity of the absorption spectra increasing with the increase of the concentration that agrees with Beer – Lambert Law. The measurement shows that the Absorption spectrum have shifted to short wavelengths (Blue Shift). Phthalocyanine molecules (CuPc) have two absorption bands in the visible and ultraviolet region of the spectrum

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INTRODUCTION

Organic compounds are defined as hydrocarbons and their derivatives. They can be subdivided into saturated and unsaturated compounds. The latter are characterized by the fact that they contain at least one double or triple bond. These multiple bonds not only have a profound effect on chemical reactivity, they also influence spectroscopic properties (Snively, 1983).

Organic compounds without double or triple bonds usually absorb at wavelength below 160 nm, corresponding to photon energy of 180Kcal/mole. This energy is higher than the dissociation energy of most chemical bonds, therefore photochemical decomposition is likely to occur, so such compounds are not very suitable as the active medium in lasers (Ponce, 2005).

The two double bonds are called conjugated. Compounds with conjugated double bonds also absorb light at wavelengths above 200nm. All dyes in the proper sense of the word, meaning compounds having a high absorption in the visible part of the spectrum, possess several conjugated double bonds. The basic mechanism responsible for light absorption by compounds containing conjugated double bonds is the same; in whatever part of the spectrum these compounds have their longest wavelength absorption band, whether near-infrared, visible, or near-ultraviolet (Macda, 1984).

Dye lasers entered the scene at a time when several hundreds of laser-active materials had

already been found. Yet they were not just another addition to the already long list of lasers. They were the fulfillment of an experimenter's pipe dream that was as old as the laser itself: To have a laser that was easily tunable over a wide range of frequencies or wavelengths. Dye lasers are attractive in several other respects: Dyes can be used in the solid, liquid, or gas phases and their concentration, and hence their absorption and gain, is readily controlled. Liquid solutions of dyes are especially convenient: The active medium can be obtained in high optical quality and cooling is simply achieved by a flow system, as in gas lasers. Moreover, a liquid is self-repairing, in contrast to a solid-state active medium where damage (induced, say, by high laser intensities) is usually permanent. In principle, liquid dye lasers have output powers of the same magnitude as solid-state lasers, since the density of active species can be the same in both and the size of an organic laser is practically unlimited. Finally, the cost of the active medium, organic dyes is negligibly small compared to that of solid-state lasers (Snively, 1983).

Experimental:

Solution of concentration for solvent is prepared by weighting an appropriate amount of the material by using a mettle balance having a sensitivity of 10^{-4} gm.

Different concentrations are prepared according to the following equation (Ali, 2009):

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

Where W weight of the dissolved dye (gm)

M_w Molecular weight of the dye (gm/mol)

V the volume of the solvent (ml)

C the dye concentration (mol/l)

The prepared solutions are 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

Apparatus used in work laboratory:

Spectrophotometer:

A UV-Visible spectrophotometer model (SP_3000), from Thermo Corporation (Optima) was used to carry out the absorption spectra. Table (1) lists the general properties of this device and Figure (1) shows a photograph of the device.

Table 1: Specifications of the Absorption Spectrophotometer.

Spectral Range	(190- 1100) nm
Scanning rate	(200, 400 & 600) nm/min
Light source	Tungsten Lamp+ Deuterium Lamp
Control	Internal Microprocessor



Fig. 1: (a photograph of the device)

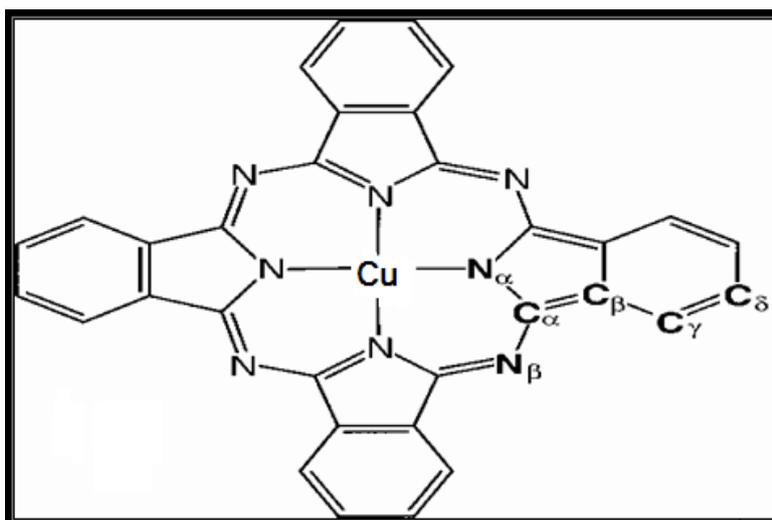


Fig. 2: Copper-Phthalocyanine molecule (Krashakov, 1984)

By using, the two lamps will be covering the (UV) and (Visible) regions of the spectrum. The principle of the work depends on the measure of comparison between the two bands, one the solvent with the solution, which is called the (Sample) and the other with the solvent alone, which is called the (Reference). The purpose of this comparison is to give the value of the dissolvent alone melted by the value of the solvent absorbance of the solution absorbance. This device is automatically programmed to carry out a survey of all the wavelengths and it shows the wavelength that gets the maximum absorption

Materials:

Chemical structure:

1- Copper-Phthalocyanine dye:

Copper-Phthalocyanine (CuPc) (~90% dye content) its molecular formula ($C_{32}H_{16}N_8Cu$) and molecular weight ($M_w=575.5$ gm. /moll) the dye being accustomed to cyanine family, are obtained from North Oil Company as in chemical formula in Figure (2).

2- The solvent: Dioxane:

The organic solvent its scientific name (1, 4 Dioxane) and molecular formula ($C_4H_8O_2$) and molecular weight (88.11 gm. /moll). In the present

investigation, we use pure Dioxane 99.99 % (spectra Grade). (Hasereg, 2005)

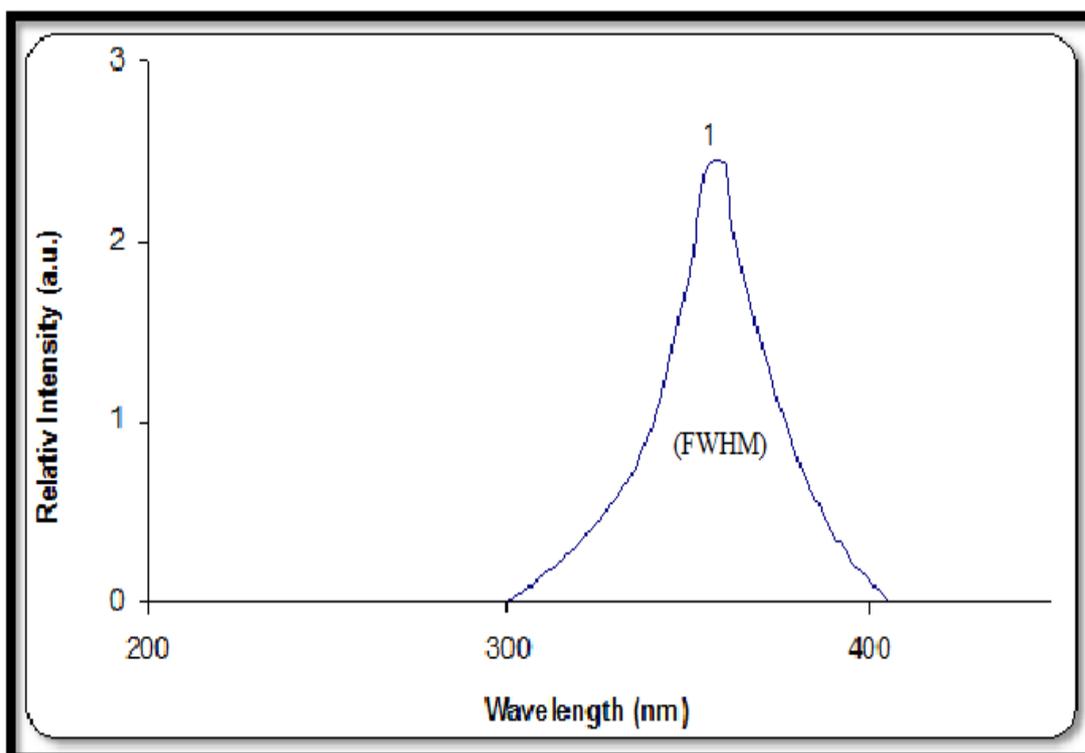
Results:

Absorption spectra in UV / Visible region around (300-700nm):

In UV region, the absorption spectrum of the Dioxane solvent as shown in figure (3) shows that the increase of the absorption intensity is varying with the increase of concentration, which is agreement with Beer-Lambert law. We observe in the absorption spectrum of CuPc dye in Dioxane as shown in figure (3) that this dye has a large absorption spectrum of wavelengths (300-420) nm, it is noted that the bandwidth of absorption spectrum in the middle intensity (λ_{FWHM}) decreases with the decrease of concentration .

It seems clearly that the effect of concentration changing in determining the maximum wavelength of absorption spectrum ($\lambda_{max,abs}$) when we have found the highest peak absorption at the wavelength (362) nm, at the highest concentration

(1×10^{-3}) M. Then this peak has been shifted towards shorter wavelengths (blue shift) exactly at (356) nm when the concentration is at (1×10^{-4}) M, then the peak is located at (352) nm, for the lowest concentration (0.5×10^{-4}) M, offsets by a decrease in the relative intensity value of the absorption, and reduces the spectrum range



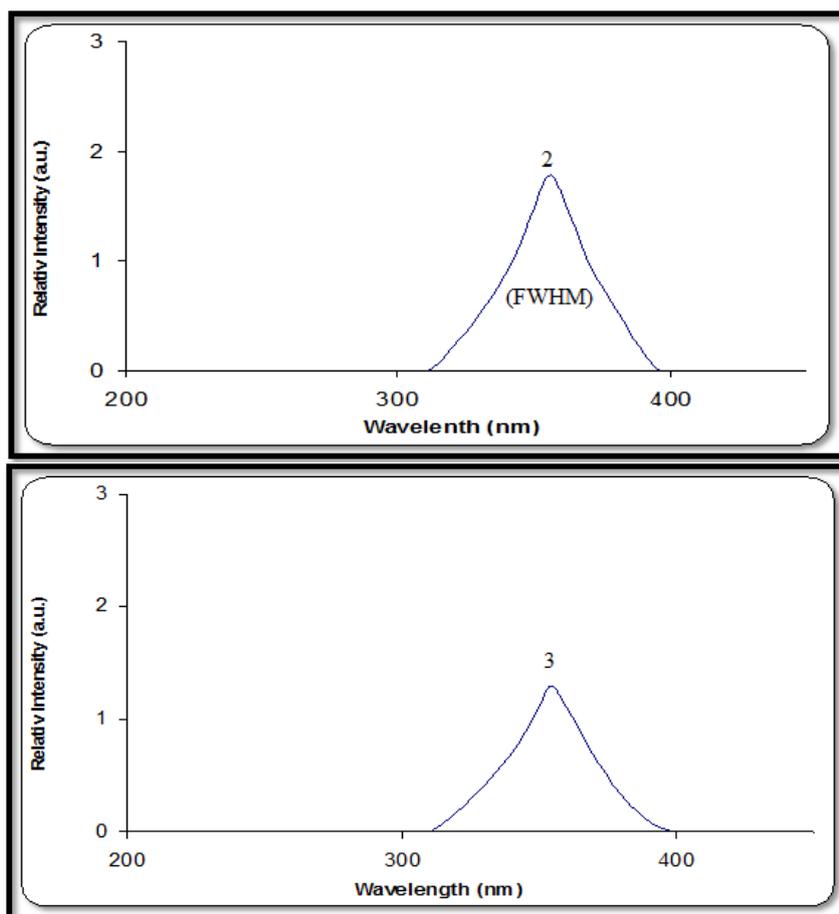


Fig. 3: Absorption spectra of CuPc dye 1×10^{-3} M (2) 1×10^{-4} (3) 0.5×10^{-4} M.

Table 2: The absorption spectra for CuPc dye in UV region.

Absorption Spectrum Dye : CuPc Solvent: Dioxane At Room Temp.				
$\Delta\lambda_{\max}$ (FWHM) (nm)	Band Width $\Delta\lambda$ (nm)	$\lambda_{\max\text{abs}}$ (nm)	Relative Intensity (a.u.)	Concentration (moll/liter)
65	106	362	2.6	1×10^{-3}
57	85	356	1.8	1×10^{-4}
38	80	352	1.4	0.5×10^{-4}

In visible region, we have observed that it has a wide range of wavelengths (580-700) nm. The peak of the absorption around (658) nm for the highest concentration is (1×10^{-3}) M, then this peak is shifted towards shorter wavelengths (blue shift) exactly at (650) nm when the concentration is (1×10^{-4}) M, then

the peak becomes at (645) nm for the lowest concentration (0.5×10^{-4}) M. This is shown in figure (4). Table (3) shows the effect of changing concentrations of Copper-Phthalocyanine dye (CuPc) on absorption spectrum.

Table 3: The absorption spectra for CuPc dye in visible region.

Spectrum Absorption Dye: CuPc Solvent: Dioxane At Room Temp.				
$\Delta\lambda_{\max}$ (FWHM) (nm)	Band Width $\Delta\lambda$ (nm)	$\lambda_{\max\text{abs}}$ (nm)	Relative Intensity (a.u.)	Concentration (moll/liter)
63	120	658	3.3	1×10^{-3}
52	100	650	2.85	1×10^{-4}
43	85	645	2	0.5×10^{-4}

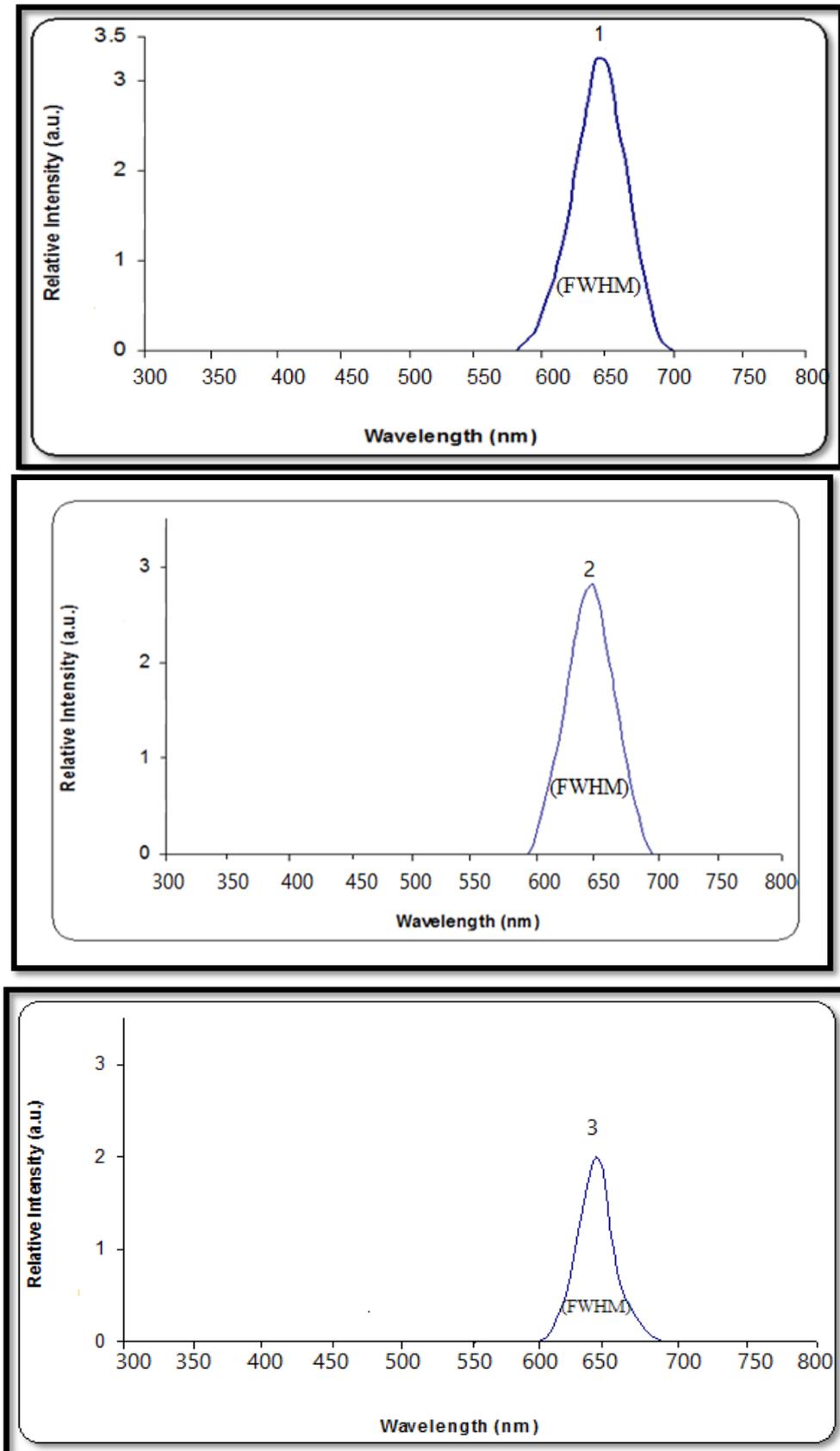


Fig. 4: Absorption spectra of CuPc dye (1) $1 \times 10^{-3} \text{ M}$ (2) 1×10^{-4} (3) $0.5 \times 10^{-4} \text{ M}$.

Discussion:

By studying the results of absorption spectra of the CuPc dye solution in the Dioxane solvent, we have observed the following :

- 1- Phthalocyanine molecules (CuPc) have two absorption bands in the visible and ultraviolet region of the spectrum. The higher energy band, occurring at around 300 nm. The lower energy band, occurring at around 700 nm.
- 2- Increasing in the intensity of absorption with increased concentration is due to the increased number of molecules, which in turn increases the probability of absorption within the concentrations used. This is agreement with Beer-Lambert law (Robert, 1987; Lu, 1986; Rohat gi 1992).
- 3- The Increase in the concentration of dye solution leads to shift a peak of absorption towards the long wavelengths (Red Shift) (because of the dipole moment of the excited state is higher than a ground state) as well as increase in the spectral rang. This is agreement with Snegov (Snegov, 1974).
- 4- We have noticed a behavior similar to the absorption spectra of the (UV) for shifting to the red region due to increase the concentration, because of the highest dipole moment of the excited state compare with ground state.

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