

# Effect of Irradiating Energy on Optical Energy Band Gap of Copper Phthalocyanine Solutions

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## Abstract

Copper phthalocyanine solution ( CuPc ) was prepared from copper phthalocyanine powder dissolved in chloroform at a concentration of (0.15 g/L) and irradiated with beta nuclear rays for beta plus(Na-22) and minus beta (Sr-90) for a period of (1 , 2 ,3)days .The optical spectra were measured before and after irradiation, for CuPC solutions .it appeared that the absorbance and reflectance were decrease with irradiating time increasing ,while the transmittance and optical energy band gap increased . Also, the optical constants such as absorption coefficient, refractive index, extinction coefficient and dielectric constant have been calculated and it was found that they were slightly depending on irradiating time.

**Keywords:** CuPc- beta ray- optical properties –optical energy band gap- IR

## 1. Introduction

Copper-phthalocyanine (Cu-Pc) is organic semiconductor P-type[1]. They are thermally and chemically highly stable [2]. (CuPc) is one of the most important colorant and has superior properties such as light fastness, resistance to alkalis and acids with tinting strength [3]

Copper phthalocyanine (CuPc) is a macrocyclic molecule consists of four isoindole units linked by four nitrogen atoms to form a conjugate structure with copper (II) ion in center. It illustrated good overall stability to organic solvents and used for the production of blue shades in most pigment consuming industries[4], it can be used in many organic applications such as field-effect devices as well as in organic solar cells in addition to many other applications.[5]. Copper phthalocyanine blue discovered wide requisitions in different fields, because of fabulous specialized properties, such as , compound sensor[6], catalysis[7], optical plate , xerography[8], non-direct optics[9], electro chromic showcase mechanisms, photovoltaic cells and photo sensitizers for photodynamic treatment . many scientists are centering their study on amalgamation of copper phthalocyanine because of its significant vitality in mechanical provisions, such as , their capability to structure , exceedingly stable metal intricate with metal cation and their force brightness and excellence of shades.the chemical strcture of CuPc as shown in figure(1)

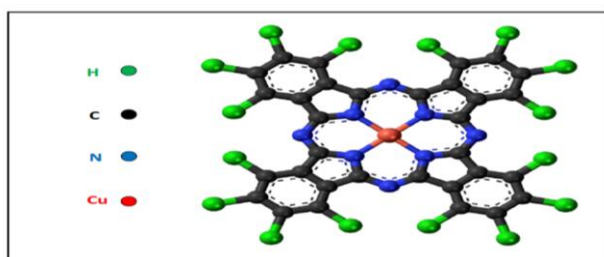


Figure 1: The Chemical Strcture Of Cupc [10]

Optical properties are important because they

provide productive means for identifying materials and are responsible for some of the properties of these materials. The interaction of light with matter when it incident, three part can be seen (IR, IT,IA) when can be obtain three spectrum , absorbance , transmittance and Reflectance spectrum. When we use the relation with Lambert equation [11]

$$I = I_0 e^{-\alpha t} \quad (1)$$

In absorbance, because molecules in the sample undergo a shift from the ground state to an excited state, the light intensity of the measurement beam decreases, as depicted by the equation:

$$A = \log \frac{I_0}{I} \quad (2)$$

the transmittance spectrum is the inverse of A , can be defined as :[12]

$$T = 10^{-A} \quad (3)$$

The reflectance spectrum is nearest to the shape of absorbance spectrum (A)can be calculated from the relation [13]

$$A+T+R=1 \quad (4)$$

The linear absorption coefficient can be calculated from relation [14]

$$\alpha = 2.303 \frac{A}{t} \quad (5)$$

t: thickness of sample

The extinction coefficient, which is proportional to the exponential decay of the wave as it goes through the medium, is defined as follows:[15]

$$k = \frac{\alpha \lambda}{4\pi}$$

The refractive index has been determined using the following expression[16]

$$n = \sqrt{\frac{4R}{(1-R)^2} - K^2 + \frac{1+R}{1-R}}$$

The material's polarization, or how it reacts to various frequencies, is represented by the dielectric constant. Real and imaginary dielectric constants ( $\epsilon_r$ ) and ( $\epsilon_i$ ) are shown in the following equations[17].

$$\epsilon_r = n^2 - k^2 \quad (8)$$

$$\epsilon_i = 2nk \quad (9)$$

The Tauc relation is used to assess whether a

transition is direct or indirect based on absorption coefficient data [18]

$$\alpha h\nu = B(h\nu - E_g)^r \quad (10)$$

Where

h: Planck's constant,

v: photon frequency,  $E_g$  : the optical energy band gap

B: a proportional constant

The value of r is 1/2 for direct band gap. the value of r is 2 for indirect

Using the following equation, the photon energy can be determined:

$$E \text{ (eV)} = h\nu = 1240 / \lambda \text{ (nm)} \quad (11)$$

the optical conductivity can be calculated from the relation

$$\sigma_{op} = \frac{\alpha n c}{4\pi} \quad (12)$$

### Experimental part

**preparation of Cupc solution** The solutions of CuPc molecules with a concentration of 0.15 g /L are prepared using chloroform as a solvent., it was irradiated in a pluse beta ray with source (Na-22) (RE 402) and half-life(2.6 year) , its manufacturing data (3/2009) with everage energy (0.544Mev) and activity (0.06 Mci). Minus beta ray source (Sr -90) (UB863) with half-life (28.8 year) and its manufacturing data (9/2012) with avarge energy (0.546 Mev )and activity (1.59Mci) in time periods ( 1, 2 , 3 )days .The optical properties and energy band gap were measured before and after irradiationn by UV-1800 Spectrophotometer Japanese made , Fourier transform infrared spectrum was measured by FTIR spectrometer IR Affinity-1 (Shimadzu Company) Japanese made . ALocal Excel software was used to calculate and plot results.

## 2. Results and Discussion

### FTIR spectra

FTIR Spectrum for CuPc powder shows that demonstrate bond bending in the range of (400-2000)  $cm^{-1}$ , and bond stretching in the range of (2000-4000)  $cm^{-1}$ . The (copper-Nitrogen) bond vibration may be seen in the region (600-400)  $cm^{-1}$ , which indicates the existence of (metal-Nitrogen) bond vibration. The C-N bond is represented by the band at (1334-1320)  $cm^{-1}$ , the C=C bond is represented by the peak at (1620)  $cm^{-1}$

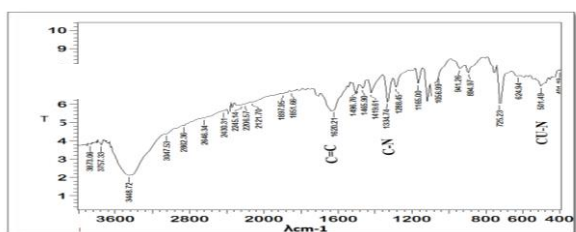


Figure 2: represent of FTIR spectrum for CuPc powder

### Absorbance

The results appeared for  $\beta$ -phase CuPc solutions when irradiated with plus and minus beta rays for several periods of time, as follows:

The relationship between the absorbance and the wavelength of CuPc solutions appeared that there are two peaks at wavelengths between (300-600nm) and the highest value is at point (358). The absorbance decreases with an increase in the wavelength of 900. The effect of the irradiation time of copper phthalocyanine solutions was shown by pluse beta rays, by increasing the irradiation time, the absorbance decreased. This can be explained by the fact that the rays broke the bonds and the molecules lost their identity.

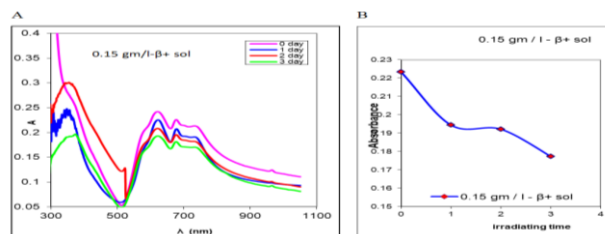


Figure 3: A. The relation between Absorbance(A) and wave length ( $\lambda$ ) for  $\beta+$  ray CuPc solution in period times. B. the relation between Absorbance and irradiating time for  $\beta+$  ray CuPc solution

Beta-minus also exhibited the same behavior, which means that nuclear rays, with both beta rays, break the covalent bonds of matter as shown figure (4)

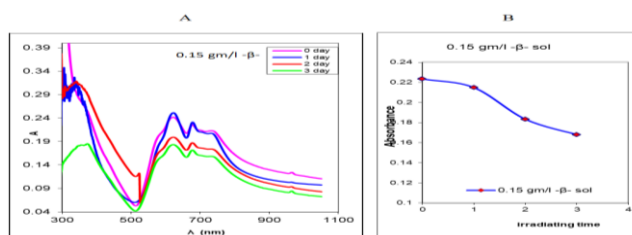


Figure 4 : A. the relation between absorbance(A) and wave length ( $\lambda$ ) for  $\beta-$  ray CuPc solution in period time . B. the relation between Absorbance(A) and irradiating time for  $\beta-$  ray CuPc solution

### Transmittance

The transmittance values were calculated from the equation(3) and their values were plotted for different irradiation times irradiated with pluse beta rays. The results showed that minum transmittance at the range the wavelength300-600 nm and gradually increase with increasing wavelength from.700-1100.nm. The relationship between transmittance and irradiation time was drawn with beta pluse rays. The results showed an increase in transmittance with increase in irradiation time with beta rays. This is due to the breakage of dye molecules as a result of irradiation

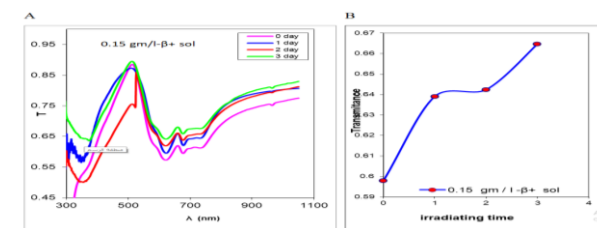


Figure 5 : A. The relation of transmittance(T)and wavelength ( $\lambda$ ) for  $\beta+$  ray CuPc solution in period time B. the relation between transmittance(T) and irradiating time for  $\beta+$  ray CuPc solution

Beta-minus also exhibited the same behavior, which means that nuclear rays, with both beta rays, break the covalent bonds of matter as shown figure (6)

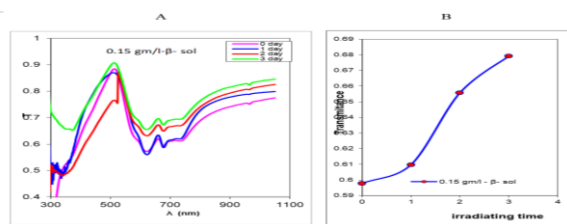


Figure 6 : A. the relation between transmittance (T) for  $\beta^-$ -ray CuPc solution in period time B. the relation between transmittance(T) and irradiating time of  $\beta^-$ -ray for CuPc solution

### Reflectance

The relationship between the reflectance and the wavelength of CuPc solutions appeared that there are two peaks at wavelengths between (300-600nm) .The reflectance decreases with an increase in the wavelength of 930. The effect of the irradiation time of copper phthalocyanine solutions was shown by plus beta rays, by increasing the irradiation time, the reflectance decreased. This can be explained by the fact that the rays broke the bonds and the molecules lost their identity.

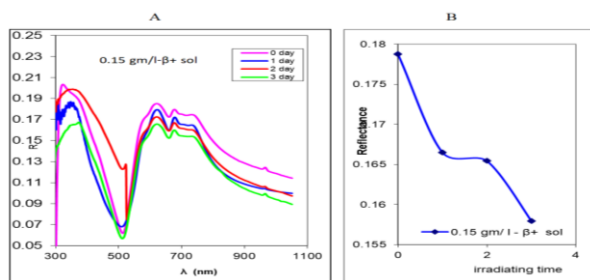


Figure 7 : A. The Relation between Reflectance (R) and wavelength ( $\lambda$ ) for  $\beta^+$  ray CuPc solution in period times B. The Relation between Reflectance and irradiating time for  $\beta^+$  ray CuPc solution.

The relationship between the reflectance and the wavelength of CuPc solutions appeared that there are two peaks at wavelengths between (300-600nm). The reflectance decreases with an increase in the wavelength of 930. The effect of the irradiation time of copper phthalocyanine solutions was shown by minus beta rays, by increasing the irradiation time, the reflectance decreased. This can be explained by the fact that the rays broke the bonds, and the molecules lost their identity as shown in figure (8)

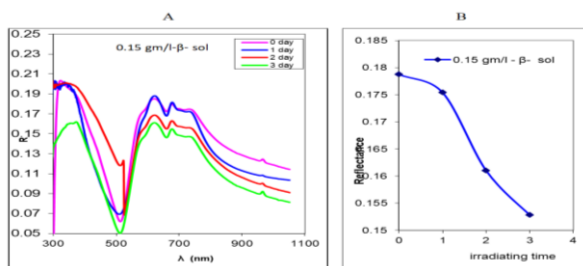


Figure 8 : A. The Relation between Reflectance (R) and wavelength ( $\lambda$ ) of  $\beta^-$ -ray for CuPc solution in period time B. the relation between Reflectance and irradiating time of  $\beta^-$ -ray for CuPc solution

### Optical Energy band gap

Beta ray due to increase of indirect optical energy band gap from 1.7 eV to 1.9 eV.

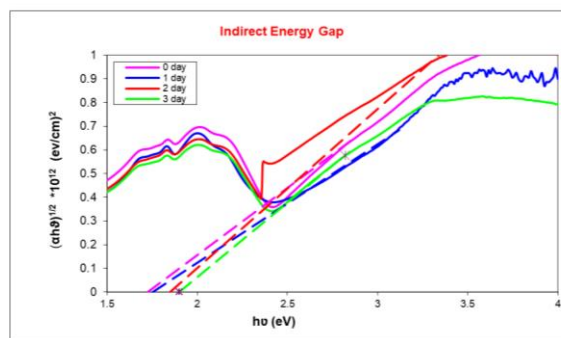


Figure 9: Determined indirect energy band gap for  $\beta^+$  ray CuPc solution in period times

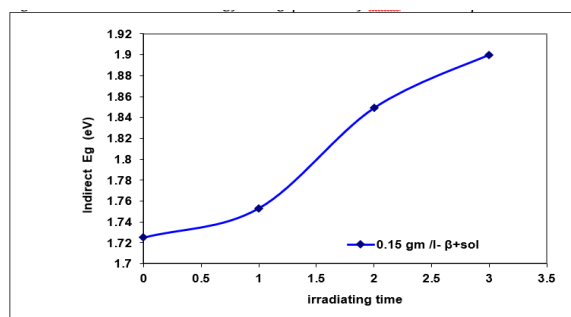


Figure 10: the relation between indirect energy band gap and irradiating time for  $\beta^+$  ray CuPc solution

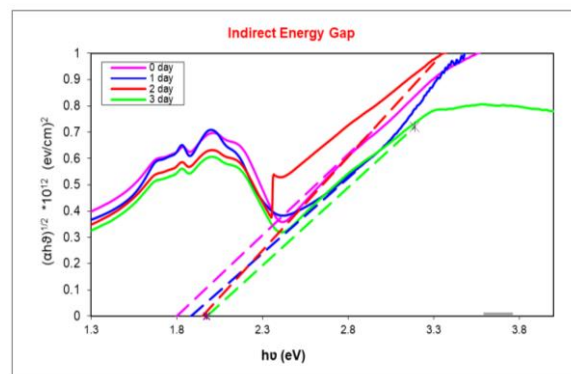


Figure 11: Determined indirect energy band gap for  $\beta^-$ -CuPc solution in period times

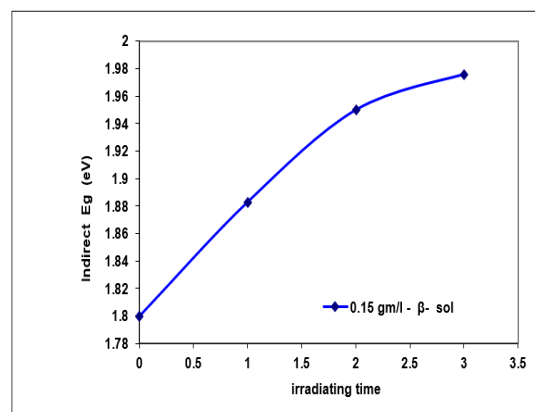


Figure 12 :The Relation between indirect energy gap and irradiating time for  $\beta^-$ -ray CuPc solution

### Optical constants

Optical constants result in Tables (1, 2)

Table 1: Optical Constants For  $\beta^+$  Cupc Sol

irradiating time day	Absorption Coefficient $\alpha$ *10 <sup>4</sup> (cm <sup>-1</sup> )	Extinction Coefficient (K)	Refractive Index (n)	Real Dielectric Constant ( $\epsilon_{Real}$ )	Imaginary Dielectric Constant ( $\epsilon_{Im.}$ )
0	0.223404023	1.06722E-06	2.305854443	5.316964711	4.92169E-06
1	0.194478404	9.29037E-07	2.206844528	4.870162771	4.10048E-06
2	0.192236438	9.18327E-07	2.189293478	4.793005934	4.02097E-06
3	0.177415488	8.47526E-07	2.125446588	4.517523199	3.60274E-06

Table 2: Optical Constants For  $\beta^-$  CuPc Sol

irradiating time day	Absorption Coefficient $\alpha$ *10 <sup>4</sup> (cm <sup>-1</sup> )	Extinction Coefficient (K)	Refractive Index (n)	Real Dielectric Constant ( $\epsilon_{Real}$ )	Imaginary Dielectric Constant ( $\epsilon_{Im.}$ )
0	0.223404023	1.06722E-06	2.305854443	5.316964711	4.92169E-06
1	0.214821544	1.02622E-06	2.285339808	5.222778037	4.69051E-06
2	0.183300277	8.75638E-07	2.151438592	4.628688013	3.76776E-06
3	0.168043417	8.02755E-07	2.082327255	4.336086796	3.3432E-06

The Linear Absorption Coefficient ( $\alpha$ ), Refractive Index (n), Real Dielectric Constant ( $\epsilon_r$ ), Imaginary Dielectric Constant ( $\epsilon_i$ ) extinction coefficient (K) are decreased with irradiating time increasing.

### 3. Conclusions

CuPc solutions effect by beta radiation, as the irradiation time increasing, the absorbance, reflectance, optical constants such as absorption coefficient, extinction coefficient, real and imaginary dielectric constant were decreased, while the transmittance and optical energy band gap increased. The energy band gap can be controlled slightly by radiation time, and this in turn affects the optical, thermal and electrical properties, since the energy gap is the factor affecting it.

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