Journal of Basrah Researches ((Sciences)) Vol. (45). No. 2(2019)

ISSN_1817_2695

Available online at: http://brsj.cepsbasra.edu.iq

Received 9-9-2019, Accepted 29-12-2019

Linear Optical Properties of a New Azo dye derived from Cefotaxime

Shaymaa H. Jasim[1*],Wisam A. Radhi[2] ,Shatha S.Ebade[1]

[1]*Department of Physics, College of Education for Pure Science, University of Basrah, Iraq*

[2]*Department of Chemistry, Polymer Research Center, University of Basrah, Iraq*

***E-Mail: Shaymaa.jasim@uobasrah.edu.iq**

Abstract

New azo dye(AZ) compound derived from (6R,7R)-3-[(acetyloxy)methyl]-7-[[(Z)-2-(2-aminothiazol-4-yl)-2-(methoxyimino)acetyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]-oct-2-ene-2-carboxylate sodium (Cefotaxime) with resorcinol, has been prepared . The Synthesis ofdye was characterized using FT-IR. Thin film of azo dye was prepared by spin coating method. The absorption spectra shows to major absorption band the first at the wavelength 323nm and the second at the wavelength 455nm. Absorption coefficients (α), refractive index (n),extinction coefficient (k) and optical band gap have been all calculated. Both refractive index(n) and extinction coefficient (k) decrease with increase of the wavelength.

Keywords: NewAzo dye,Optical Properties,Cefotaxime.

1. Introduction

Cefotaxime(CFX)is classed as a third-generationbactericidal of cephalosporin. Regarding its antibacterial activity, Cefotaxime has been found to possessdifferent degrees of activity against

Gram-positive and Gram-negative bacteria [1].

Chemical connection between azo groups (–N=N–) and SP^2 hybridized carbon atoms lead to create azo compounds [2, 3]. Azo dye has received great attention due to its environmental stability, ease of preparation, and its optical and electrical properties. Furthermore, the molecular design, synthesis, and assembly of structures with desired properties were received the attention of researchers [4, 5]. azo dyes have a wide spectrum of industrial applications such as food, wool, polymeric fibers, conductive textile and optical properties [6-9]. These compounds have utilized in diverse applications such as polarized photoinduced anisotropy, nonlinear optics effect and all-photoswitching.

Optical constants of materials such as refractive index and extinction coefficient are considered a criticalsubstantial to examine material's potential optoelectronic applications [10]. Further, optical properties could be closely related to the material's atomic structure, electronic band structure and electrical properties. The optical properties have a vital role in optics applications such as optical modulation, optical information, optical data and integrated optics. The optical properties of a material can be modified by control of characteristics of the passing light [7]. Studies have indicated that most important optical properties of the substances are absorption coefficient, refractive index and extinction coefficient.In this study, a new compound of azo dyes has been derived from(6R,7R)-3-[(acetyloxy)methyl]-7-[[(Z)-2-(2-aminothiazol-4-yl)-2-(methoxyimino)acetyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]-oct-2-ene-2-carboxylate sodium. The optical constants, particularly the refractive index and the absorption coefficient, of the prepared dyes have been measured.

2. Experimental

2.1. Preparation of azo dye compound

Based on Fox method [12], azo dyes have been prepared. Firstly, (0.0025mole, 1.193g) of (CFX) has been dissolved in 2ml of concentration hydrochloric acid. After adding 10ml of distilled water, the mixture has been stirred before keeping it in an ice bath. After being prepared by dissolving 0.456g of sodium nitrite in around 5ml of distilled water and kept in an ice bath, the resultant diazonium salt has added as drop wisely to the mixture (CFX) at temperature range of 0-5 ^{o}C. The next step is to prepare a coupler by dissolving (0.0025mole, 0.275g) of resorcinol in 25% sodium hydroxide solution and keeping the mixture in an ice bath. By keeping the temperature below 5o ^{o}C, the diazonium salt has been added dropwisely to the couplers with constant stirring. To neutralize the dyes, a diluted solution of hydrochloric acid has been added. The dark red azo dye was then collected and washed with cold water recrystalized from methanol yielded the pure azo dye(Amorphous powder). Figure (1) shows the chemical structure of the azo dye compound. The physical properties of the azo dye compound are given in table (1).

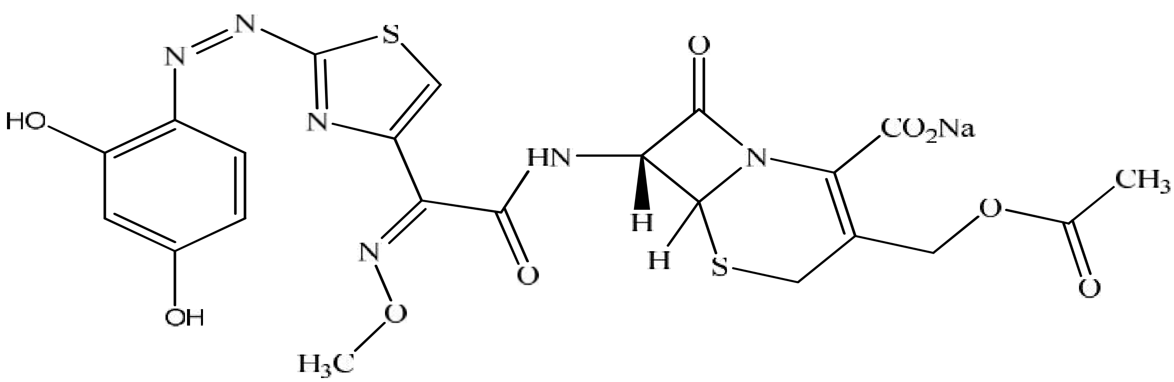

Figure 1: Chemical structures of azo dye compound

Table 1: show physical properties of azo dye compound

compound	Yield (%)	M.P(^{o}C)	Color	Formula
CFX	/	/	White	$C_{16}H_{16}N_5NaO_7S_2$
AZ	70	>250*	dark red	$C_{22}H_{19}N_6NaO_9S_2$

* = decomposition

2.2. Preparation of thin film and instruments

A thin film of azo dye has spin coated at 2500 rpm on a glass substrate of 2.2cm×2.2 cm. The coated film has been kept to dry at room temperature for 24 hr. To evaporate any remaining solvents, the film has been heated gradually from room temperature to 80 ^{0}C for 2 hr. The film thickness has been found to be about 379nm calculating by using equation (1). [13]

$$t = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)} \qquad (1)$$

Ifn1 and n2 are the refractive indices at two adjacent maxima (or minima) at λ1 and λ2.

The absorption (A) and transmittance (T) have been investigated in the range of wavelength (300 – 900) nm. The measurements have been taken by double beam UV-visible spectrophotometer (UV-1800) at room temperature.

3. Results and Discussion

3.1. FT-IR Spectra

The FT-IR spectrum of the prepared azo dyewas recorded as KBr diskusing Jasco(4200) –USA apparatus in rang (4000-400cm^{-1}).The spectral data of the product was gathered in figure (2) and Table 2: The azo

dye(AZ) exhibited intense IR absorptions at 3241cm^{-1} [ν(O-H)] , 2950 cm^{-1} [ν(C-H aliphatic)] , 1743cm^{-1} [ν(C=O) lactam] , 1622 cm^{-1}[ν(C=C)] , 1443 cm^{-1} [ν(-N=N-)] [14], 1040cm^{-1} [ν(C-O)].

The FT-IR spectrum of compounds is listed in table (2). The IR spectrum of amine which is shown in figure (3) contain characteristic bonds at around (3463,3345cm^{-1}), (1760cm^{-1}), (1730cm^{-1}) due to υ(NH), υ(C=O) lactam, and υ(C=O) ester respectively.

Table .2 Major IR absorption bands (cm^{-1}) of CFX and Azo dye

Comp.	ν (O-H)	ν (N-H)	ν (CH) aliphatic	ν (C=O) lactam	ν (C=O) ester	ν (C=C)	ν (N=N)	ν (C-H) aliphatic (bend)	ν (C-O)
CFX	/	3463,3345 br	2938 (w)	1760 (s)	1730 (s)	1649 (s)	/	1387 (s)	1045 (s)

AZ	3241 (br)	/	2950 (w)	1743 (s)	/	1622 (s)	1443 (s)	1384 (s)	1040 (s)

br = broad , m= medium , S= strong, W= weak

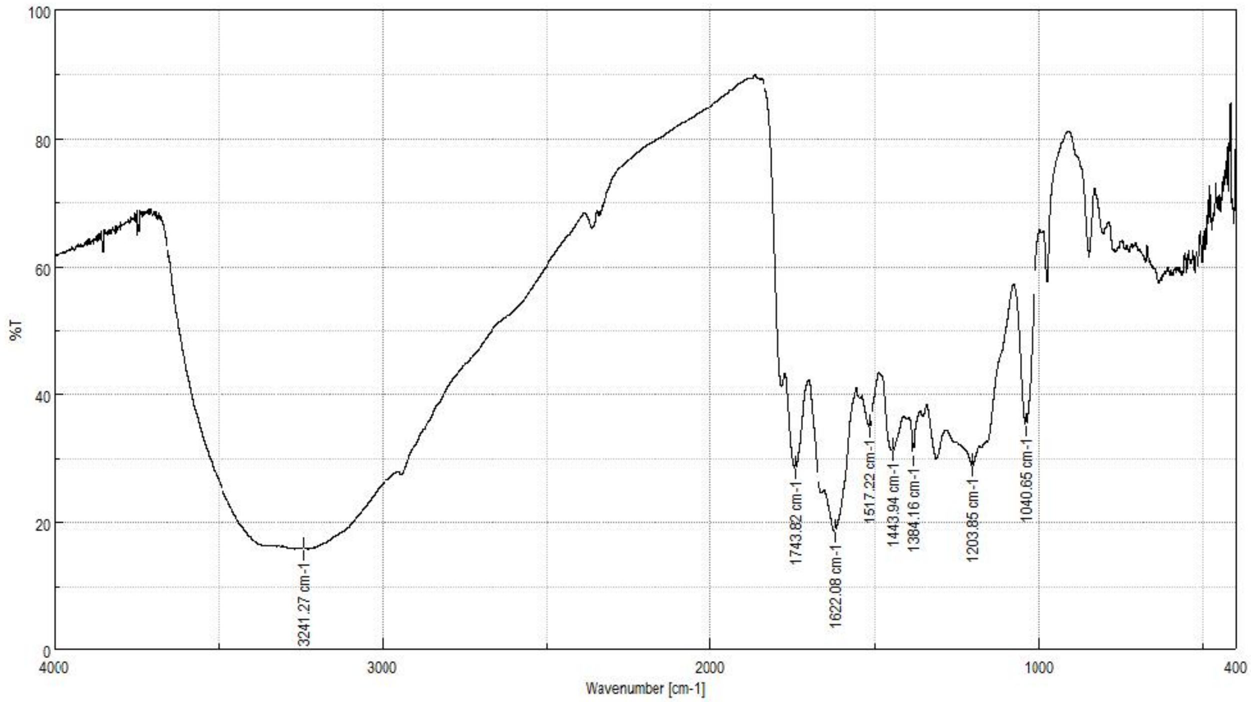

Figure 2. IR spectrum of AZ dye

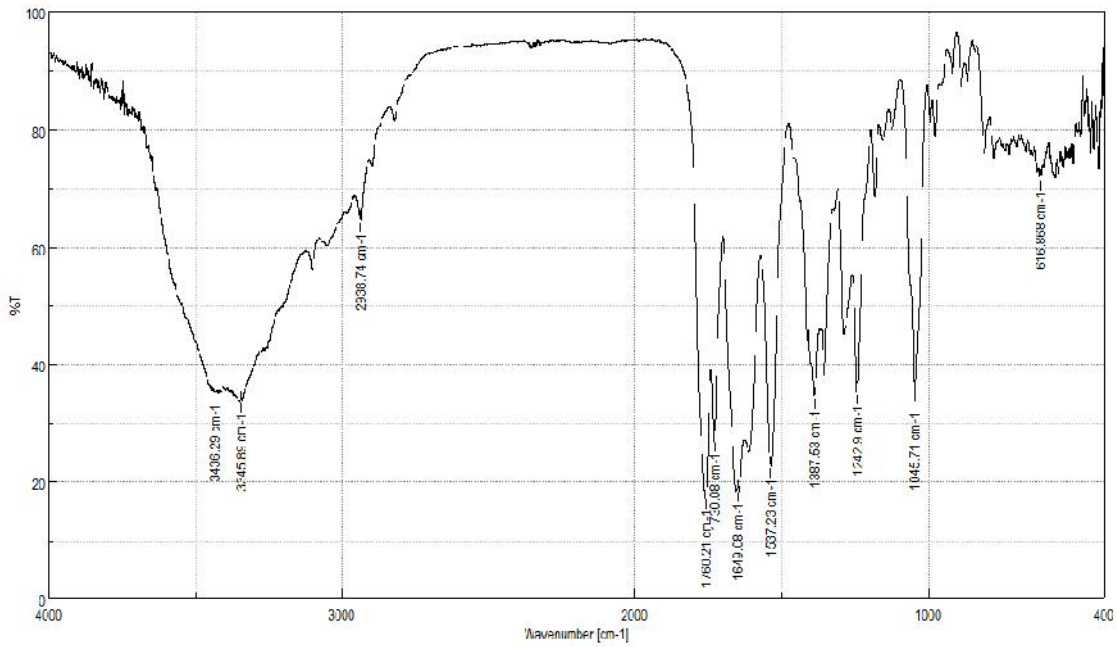

Figure 3. IR spectrum of CFX

3.2. Optical parameters measurements

Figure (4) shows the optical absorbance (A) versus the wavelength(λ) of the incident light on the prepared azo compound thin film in the wavelength range (300-900) nm. It is obvious that there are two absorption bands. An intense absorption band in ultraviolet region (wavelength 323nm) followed by a less intensity absorption band in the visible region (wavelength 455nm). The first absorption band may be attributed to σ-σ* transitions, while the second band attributed to π-π* transitions.

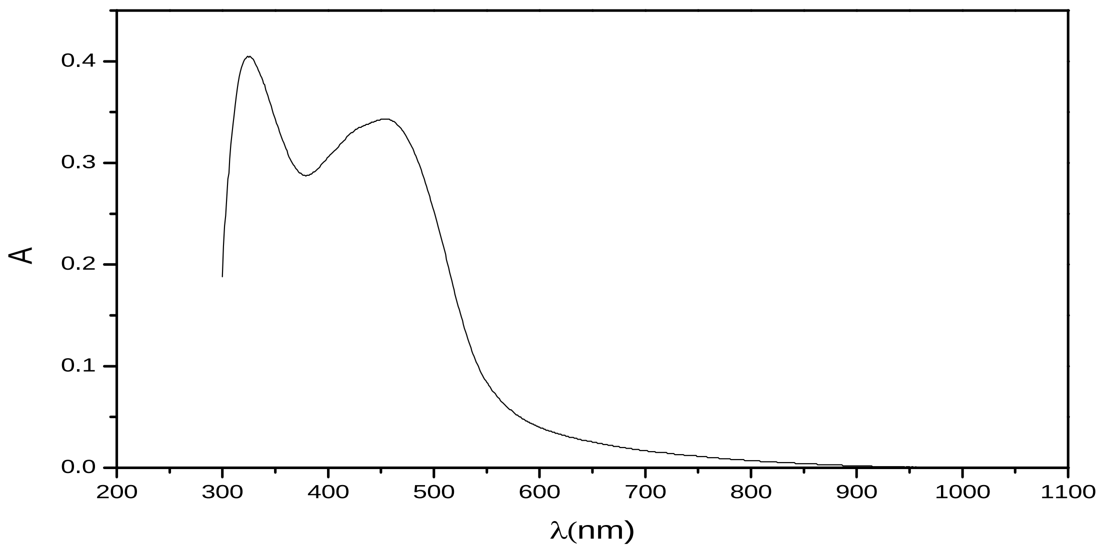

Figure 4. Absorption spectra of azo dye film

The transmittance (T) of the prepared azo compound thin film as a function of wavelengths was recorded by the spectrophotometer mentioned. Previously, and the reflectance(R) values were calculated according to the equation (2) [15]:

$$R = 1 - \sqrt{\frac{T}{e^{-A}}} \qquad (2)$$

Figure (5) shows both the transmittance (T) solid line and the reflectance (dot line) as a function of wavelengths.

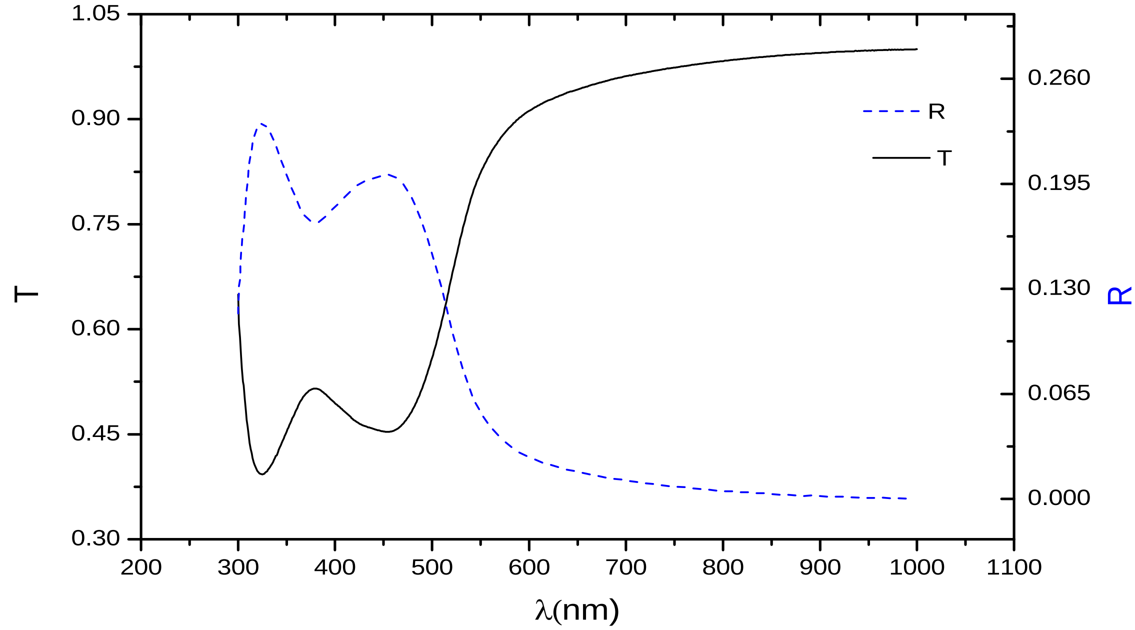

Figure 5. The spectral distribution of transmittance (T) and reflectance (R) as a function of wavelength for azo dye film.

The absorption coefficient (α) as function of the incident photon energy (hυ) is depicted in figure (6). Absorption coefficient values were calculated according to the equation (3) [16]:

$$\alpha = \frac{2.303\,A}{d} \qquad (3)$$

Where, d, is the thickness of the prepared azo compound thin film. It can be seen from figure (6) that α increase with increase of photon energy due band transition and that $\alpha > 10^4$ cm^{-1}i.e the electron transition from valance band to conduction band is direct transition [17]:

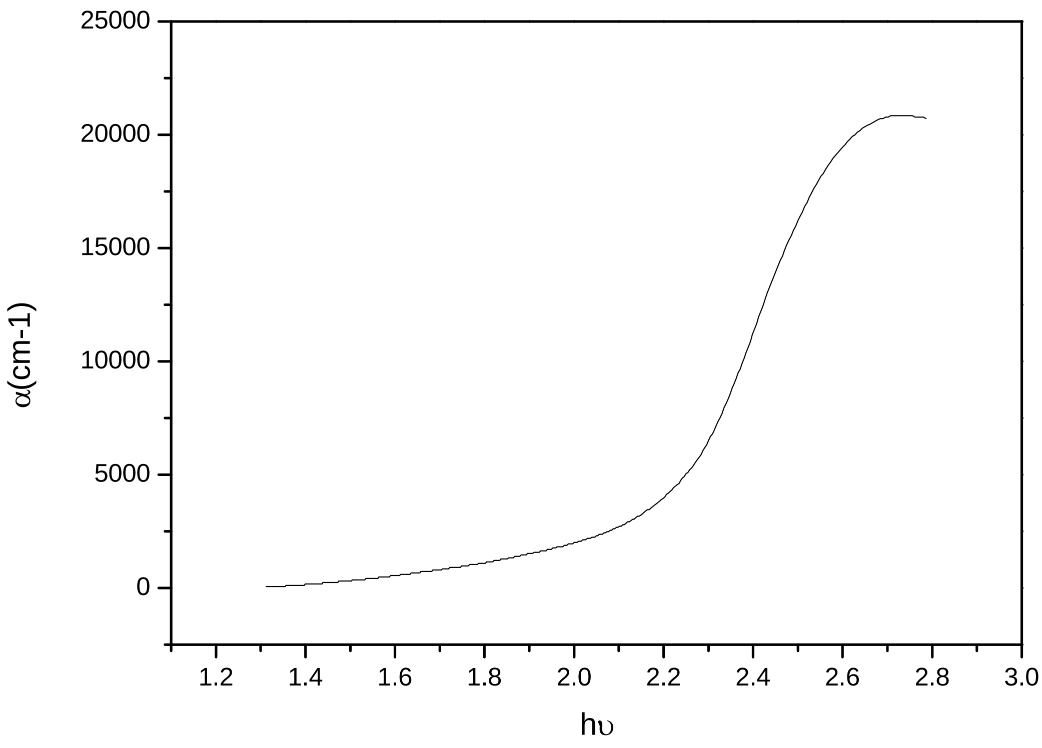

Figure 6. Absorption coefficient α(cm^{-1}) as a function of photon energy(*hυ*)

The extinction coefficient (K) depends on the absorption coefficient and can be obtained at various wavelengths using the equation (4) [18]:

$$K = \frac{\lambda\alpha}{4\pi} \qquad (4)$$

The extinction coefficient values as a function of wavelength is depicted in figure (7). The relativity high attenuation (lose of energy) of the incident light nearer to shorter wavelengths may be related to generation of phonos, scattering or photo generation.

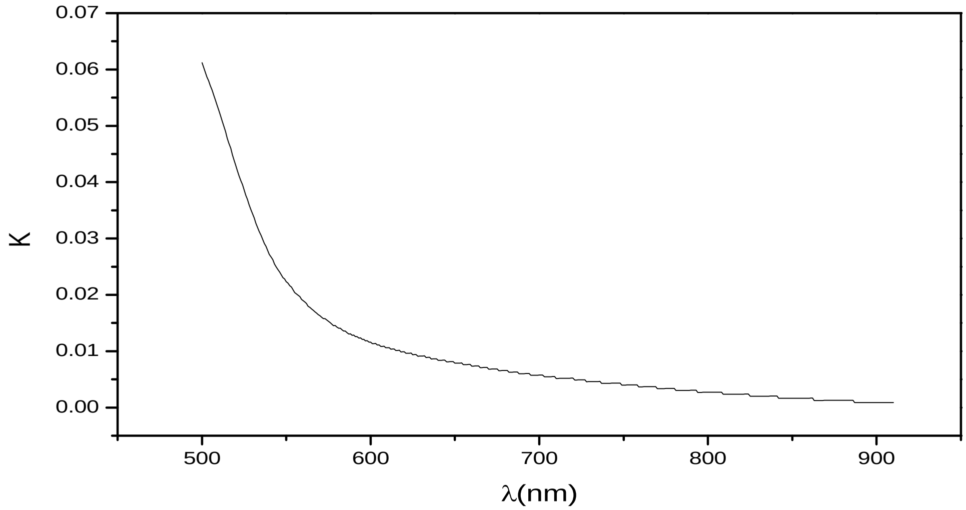

Figure 7. Extinction coefficient as a function of wavelength for azo dye film.

The refractive index values which were calculated according to the equation (5) [19]:

$$n = \left(\frac{1+R}{1-R}\right) + \sqrt{\frac{4R}{(1-R)^2} - k} \qquad (5)$$

Is plotted against the incident light wavelengths as shown in figure (8). Relativity high refractive index(n) nearer to short wavelength, corresponds to direct band to band transition of electrons.

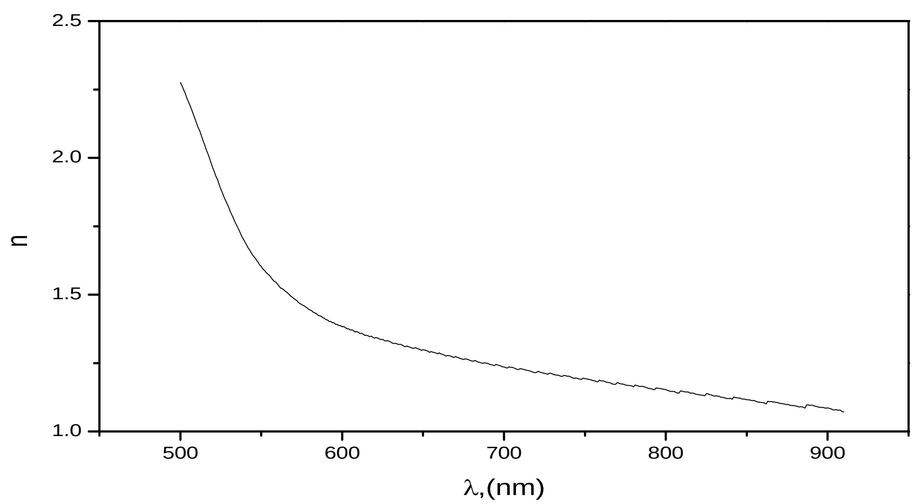

Figure 8. Refraction index as a function of wavelength for azo dye film

The optical band gap was analyzed using the equation (6) [20]:

$$(\propto h\upsilon) = B(h\upsilon - Eg)^m \qquad (6)$$

Where B is constant, h is Planck's constant, υ is the frequency of the incident light, *hυ* is the photon energy, Eg is the optical band gap, m=1/2 for direct transition. A plot of $(\alpha h\upsilon)^2$ values against photon energy (*hυ*) for the prepared azo compound thin film is shown in figure(9). The band gap (Eg) value are evaluated after extra polating the straight line portion of the curve to $(\alpha h\upsilon)^2$= 0 and found to be 2.29 eV. This explains the absorption peak in the visible region of absorption spectra. The obtained value of the azo dye Eg which is (2.29eV) may put this material as to be belong to semiconductor type of material.

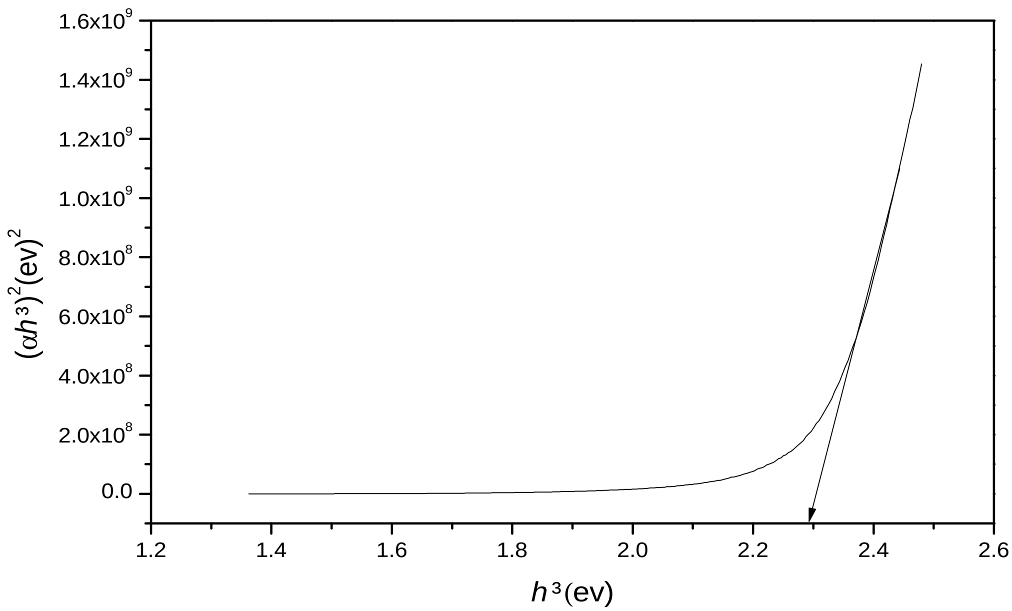

Figure 9. Dependence of $(\alpha h\upsilon)^2$ on the photon energy.

Conclusion

The optical constant of the prepared azo compound (n,k) decrease with the increase of wavelength, and the optical band gap was found to be 2,29 eV, which mean that this azo dye may behave like organic semiconductor. It is found that α values bigger than 10000, which mean the transition of electron from band to band is direct transition.

References

1. G. M. Pacifici1, G. Marchini,***International Journal of Pediatrics***,5(11),611,**(2017).**

2. H. A S. A Majeed, A. Y. Al-Ahmad and K. A. Hussain, ***Journal of Basrah Researches ((Sciences))***, 37(2),64,**(2011).**

3. H.M Ali, S. Q. Badr, A.A Saleh, H. A S .A Majeed and A. A .Hussain, ***Research Journal of Pharmaceutical, Biological and Chemical Sciences***, 10(1),1454,**(2019)**.

4.H. A. BADRAN, A. Y. TAHA, A. F. ABDULKADER, C. A.EMSHARY, ***Journa of Ovonic Research***,6(8),161,**(2012)**.

5. S. Yin, H.Xu, W.Shi ,Y.Gao, Y.Song, J.W.Y. Lam , B.Z.Tang , ***Polymer*** ,46, 10592,**(2005)**.

6. L. Change and T. Root, ***J. Am. Chem. Soc***., 126, 12, 16302,**(2004)**.

7. M. Lee and Z. Medaik, ***Chem. Mater***., 15, 2766,**(2008)**.

8. R. Serreno and D. Lydenst, ***Coord. Chem. Rev***. 276, 195,**(2007)**.

9. A. Hudson and P. Nejy. ***Acta. Chem. Slov***. 56, 833,**(2006)**.

10.M. Dongol, .***Egypt. J. Sol.***,25,33,**(2002)**.

11. Yin M,Li HP, Tang SH and Ji W, ***Applied Phys. B-Laser and Optics***,70,587,**(2000)**.

12. J. J. Fox, ***J. Chem. Soc***, 97, 1339, **(1910)**.

13. A. M. Bakry, ***Egypt. J. Solids***, 31(1),11,**(2008)**.

14. K . Nakanish and P.Solomon." *Infrared AbsorptionSpectroscopy "* . HOLDEN – DAY , Inc.,London , Sydeny,**(1977)**.

15. M. A. Nattiq, ***Journal of Basrah Researches ((Sciences))***,40 (1),28,**(2014)**.

16. O.G. Abdullah, B. K. Aziz, and S. A. Hussen, ***Chemistry and Materials Research,***3 (9), 84,**(2013)**.

17. W.A. Radhi, M. T. Obeed and S. H. Jasim and A.A.Hussein, ***Journal of Basrah Researches ((Sciences))***,42, (2),35,**(2016)**.

18. Z. T.Khodair, M. H. Saeed and M.H. Abdul- Allah, ***Iraqi Journal of Physics,*** 12, 24, 47,**(2014)**.

19.H. A. Badran · A. A. Al‑Fregi · R. K. Fakher Alfahed · A. S. Al‑Asadi,***J Mater Sci: Mater Electron,***28(22),7661,**(2017)**.

20. R. K. F.Alfahed, A. S. Al‑Asadi · H. A.Badran, K I. Ajeel,Applied Physics B,125(48),7154,**(2019)**.

الخواص البصرية الخطية لصبغة ازو جديدة مشتقة من السيفوتاكسيم

[1]شيماء هاشم جاسم،[2] وسام عبد الحسن راضي،[1]شذى سامي عبادي

[1] قسم الفيزياء، كلية التربية للعلوم الصرفة، جامعة البصرة، العراق

[2]قسم الكيمياء، مركز ابحاث البوليمر، جامعة البصرة ، العراق

***E-Mail:** Shaymaa.jasim@uobasrah.edu.iq

الخلاصة

تم في هذا البحث تحضير صبغة ازو جديدة من المركب(6R,7R) اسيتايلوكسي مثيل –7–(Z) (2)––2امينوثايازول 4– بل)–2–(ميثوكسيامينيو)اسيتايل)امينو 8–اوكسو–5–ثايا–1–ازاباي سايكليو(4.2.0) اوكتو2–ين–2–كاربوكسيلات الصوديوم مع الريسوسينول .شخصت الصبغة المحضرة بواسطة طيف الاشعة تحت الحمراء . كما تم تحضير الغشاء الرقيق لمركب الصبغة المحضرة باستخدام تقنية طلاء البرم. كما استخدم جهاز (UV) من نوع (CE 7200) ضمن مدى الاطوال الموجية (300-900) نانومتر للقياس . حيث لوحظ في اطياف الامتصاص حزمتي امتصاص تقع الاولى عند الطول الموجي (323nm) والثانية عند الطول الموجي (455nm) .كماشملت الدراسة على حساب معامل الامتصاص (α) ومعامل الانكسار (n) ومعامل الخمود (k) وفجوة الطاقة (Eg) حيث لوحظ ان قيم معامل الامتصاص اكبر من 10000 حيث يعتبر هذا النوع من الانتقالات المباشرة . كما ان قيم معامل الانكسار ومعامل الخمود تتناقص مع زيادة الطول الموجي .

الكلمات المفتاحية: صبغةازوجديدة،الخواصالبصرية،السيفوتاكسيم.