The Effect of Anthracene on Optical Properties of Polycarbonate Films

[1]Asrar Abdulmunem Saeed, [2]Mahasin F. Hadi Al- Kadhemy and [3]Zainab Jasim Neamah

[1,2]Al- Mustansiriyah Univ. - College of Science – Physics Department
[3]College of Education for Pure Science- Ibn Al-Haitham - Baghdad University

[1] asrarabdulmunim@yahoo.com
[2] drmahasinf@yahoo.com [3]ajajh02@gmail.com

Abstract

Films of pure and doped polycarbonate (PC) with different doping ratio of anthracene were prepared using casting method, in order to research the effect of anthracene additions on the optical properties of PC hosts. These films were described using UV/VIS technique in order to assessment the type of transition which was found to be indirect transition. The optical energy gap of polycarbonate (PC) was (4.43eV) and after doping PC polymer with anthracene the energy gap doesn't change significantly. Absorption coefficient, refractive index and extinction coefficient affects by doping.

Key Words: Optical properties, Anthracene, Polymer, Polycarbonate, Effect of Doping ratio.

تاثير الانثراسين على الخصائص البصريةلاغشية البولي كاربونيت

[١]اسرار عبد المنعم سعيد, [٢]محاسن فاصل هادي الكاظمي و [٣]زينب جاسم نعمه

[١و٢]الجامعه المستنصريه – كليه العلوم – قسم الفيزياء

[٣]كليه التربيه للعلوم الصرفه – ابن الهيثم – جامعه بغداد

الخلاصه

اغشية البولي كاربونيت النقيه والمطعمه مع نسب مختلفه من الانثراسين قد تم تحصيرها بطريقه الصب من اجل التحقق من تاثير اضافه الانثراسين على خصائص البصرية لمضيف البولي كاربونيت . هذه الشرائح قد تم وصفها باستخدام UV/VIS من اجل تقييم نوع الانتقال والذي وجد انه انتقال غير مباشر. فجوه الطاقه البصريه لبولي كاربونيت (٤.٤٣الكترون فولت) وبعد

تطعيم البولي كاربونيت مع الانثراسين فان فجوه الطاقه لاتتاثر بشكل كبير. معامل الامتصاص و معامل الانكسار و معامل الخمود سوف تتاثر بواسطه التطعيم.

الكلمات المفتاحيه: الخصائص الفيزيائيه, الانثراسين, البوليمر, البولي كاربونيت, تاثير نسبه التطعيم.

1. Introduction

The study of optical properties of materials is very important because the used of materials in optical application wanted exact information of their optical constant over a wide range of wavelengths [1].

Polymers are a wide class of materials which are made from repeating units of smaller molecule called monomers. Polymers are advantageous because of their strength and durability in many applications [2]. Organic and inorganic fillers like pigments, short fibers, long fibers, paper and fabrics can be incorporation into polymer matrix to enhance the physical properties of polymer to specific application [3].

Polycarbonate is a kind of polyester where the carbonate ester groups have been connected with aromatic groups, this structure gives a material resistance to high temperatures [4]. Polycarbonate (PC) exhibit a unique combination of properties such as excellent toughness compared to other thermoplastic, high transparency and dimensional stability over a wide temperature ranges. It usually used as a lighter and tougher substitute for glass or metal [5].

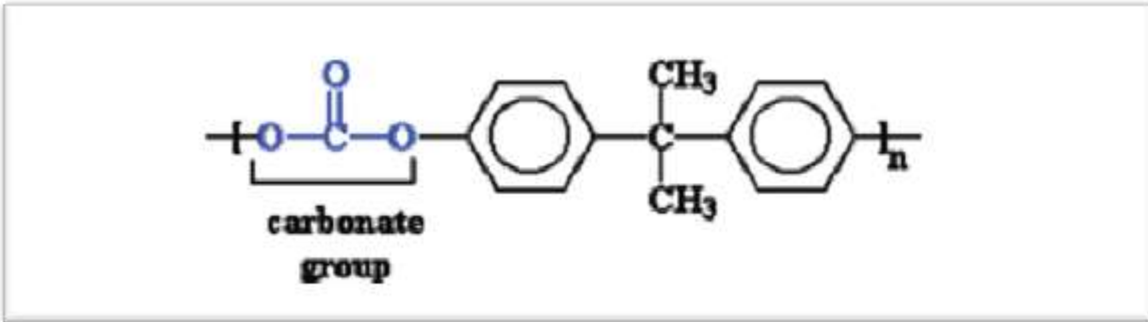

Figure (1) Polycarbonate structure [4]

The relationship between the intensity of incident and transmitted light is given by the equation [6]:

$$I = I_o \, e^{-\alpha t} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

Where (I_o) and (I) are the intensities of the incident and transmitted light, respectively,(α) is the optical absorption coefficient, (t) is the thickness of film and absorbance is defined by $A=\log (I_o/I)$.

The optical absorption coefficient (α) can be calculated from the optical absorbance spectra by using the relation [6]:

$$\alpha t = \log\left(\frac{I_o}{I}\right) = 2.303A \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

The extinction coefficient (K) is related to absorption coefficient (α), by the following equation [7]:

$$K = \frac{\alpha\lambda}{4\pi} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Where, λ is the wavelength of incident light.
The reflectance (R) can be calculated from the values of the absorbance and transmission coefficient from the equation [8]:

$$R = 1 - (A + T) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

The refractive index (n) depends on the reflectance (R) and extinction coefficient (K) and it can be calculated from the following equation [9]:

$$n = \sqrt{\frac{4R}{(R-1)^2} - K^2} - \frac{(R+1)}{(R-1)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

The absorption edge for direct and indirect transition can be obtained in the view of the proposed by Tauc et al. [10]

$$\alpha h\upsilon = A(h\upsilon - E_g)^r \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Where (h υ) is the energy of photon, (A) is the proportional constant, (E_g) is the allowed or forbidden energy gap of direct and indirect transition and(r) is constant depended on the electronic transition, r=1/2, 3/2, 2 or 3 for allow direct, forbidden direct, allow indirect and forbidden indirect transition, respectively.

The Dielectric constant clarified the ability of material to polarization and can be express by the following equation [8]:

$$\varepsilon = \varepsilon_r - \varepsilon_i \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

The dielectric constant is divided into two parts real (ε_r) and imaginary (ε_i) and described by the following equations [8]:

$$\varepsilon_r = n^2 - K^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

$$\varepsilon_i = 2nK \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

H. M. El Ghanem et al [11] studied the electrical and optical properties of polycarbonate/$MnCl_2$ composite thin films with thickness (0.2 mm) which prepared by casting technique. The optical energy gap of polycarbonate is (4.45eV) and decreased in polycarbonate/$MnCl_2$ composite with increasing the content of $MnCl_2$.

N. J. Hameed. & M. R. Fraih [12] studied the optical constants of the PMMA/PC blends. The samples are casted as films from the PMMA and PC homopolymers and blend. The energy gap for PMMA is (5 eV) and the energy gap for PC is (4.25 eV). The energy gap of 50% PMMA/ 50% PC (2.5 eV) which is less than the energy gap of PC and PMMA and the other binary blends.

The aim of the present work is to concern with the investigation the optical properties of pure PC and doping PC with anthracene with different doping ratio (10, 20, 30, 40, 50and 60) ml.

2. Experimental Work

Anthracene processed by the company chemical point, Germany, has chemical formula $C_{14}H_{10}$ and molecular weight (M_w=178.23 g/mol). Polycarbonate polymer has been choosing as host material for anthracene due to its excellent optical properties. Polycarbonate processed by the company Sabic, with molecular formula $[C_{16}H_{14}O_3]_n$ and the common brand name Lexan.

The cast technique was used to prepare the pure PC and anthracene doping PC films. PC solution is prepared by dissolved (0.3g) of PC in (10 ml) chloroform. The PC solution is stirred very well at magnetic stirrer until polymer is dissolve and cast onto glass petri dish with diameter (10 cm) and then leave it dry at room temperature about(25-30)°C for 24hr. Anthracene solution with concentration ($1x10^{-4}$ mole/liter) is prepared according to the method mentioned in ref.[13]. Then, different ratio of anthracene solution (10, 20, 30, 40, 50 and 60) ml were added to PC solution and mixed very well by use magnetic stirrer. The mixture cast onto glass petri dish with (10cm) diameter and left to dry at room temperature for 24 hr to get homogeneous films. The UV-VIS spectrophotometer type (T70/T80 Series UV/VIS Spectrometer) used to measure the absorption and transmission spectra in the wavelength range (200-900) nm.

3. Results and Discussions

In this section, absorption spectra of anthracene in chloroform solution, pure PC film, PC/anthracene films and all optical properties of samples are demonstrated.

3.1 Absorption Spectrum of Anthracene in Chloroform Solution:

Figure (2) shows the absorption spectrum of anthracene in chloroform solution with concentration ($1x10^{-4}$) mole/liter. The absorption spectrum has five peaks, the first peak appear at wavelength (310nm) with intensity(

0.1), the second peak at wavelength (325nm) with intensity (0.216), the third peak at wavelength (340nm) with intensity (0.379), the fourth peak at wavelength (360nm) with intensity(0.63), and fifth peak at wavelength(380nm) with the intensity (0.488). These peaks are due to π→π* electronic transitions this is agree with J. Kunnil et al [14].

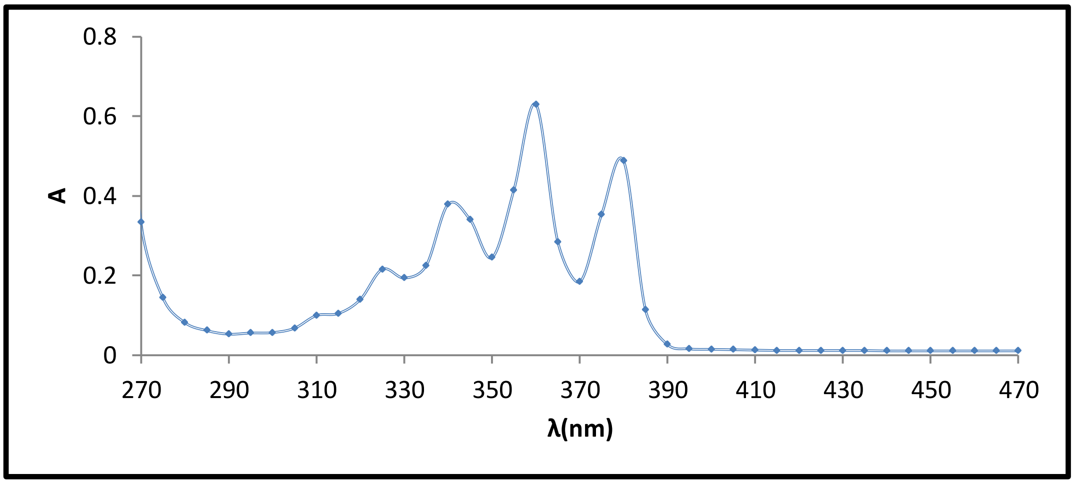

Figure (2) Absorption spectrum of anthracene in chloroform solution

3.2 Absorption Spectrum of Pure Polycarbonate Film:

The absorption spectrum for pure polycarbonate (PC) is shown in the figure (3), the absorption spectrum is broad band with two peaks the first peak at wavelength (305nm) with intensity (0.638) and the second peak at wavelength (345nm) with intensity (0.609). The different between two peaks is (40nm) which refer to the same formation origin so these two peaks are due to the n→π* and π→π* electronic transitions of the carbonyl group this agree with S. Gupta et al [15].

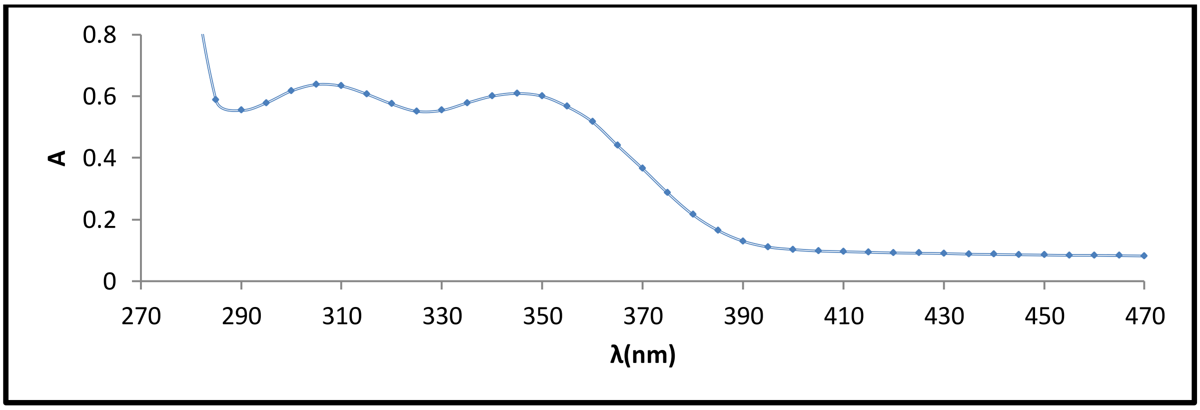

Figure (3) Absorption spectrum of polycarbonate PC film

3.3 Absorption Spectrum of Anthracene Doping PC Polymer Films:

The absorption spectrum for pure polycarbonate film and anthracene doping polycarbonate films for different doping ratio (10, 20, 30, 40, 50 and 60) ml is shown in the figure (4). In anthracene doping polycarbonate films, the intensity of the first peak of polycarbonate (310nm) increased for doping ratio (10ml) of anthracene and then decrease with increase the doing ratio. The intensity of the second peak of polycarbonate (345nm) increased with increasing the doping ratio till (50ml) then the intensity decrease. For peak (360nm) which appears after doping ratio (20ml), the intensity of this peak increase with increase the doping ratio till (50ml) then the intensity decrease. The intensity of peak (380nm) which appears after doping ratio (30ml) increase for doping ratio (40ml) and then the intensity decrease for doping ratio (50ml) and (60ml). Also, figure (3) show that the role of polycarbonate decrease with increase the doping ratio ; this is due to increase the number of anthracene molecules that is denominate and decrease the role of polymer.

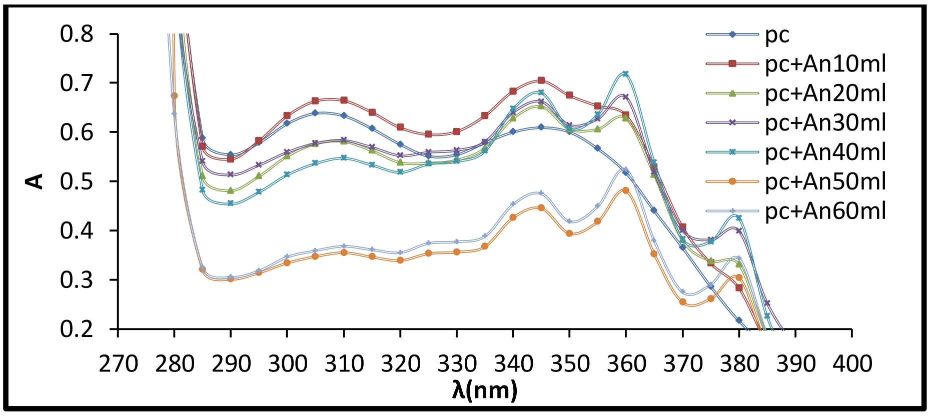

Figure (4) Absorption spectrum of anthracene doped PC films in different doping ratio

3.4 Transmission Spectrum

The spectral transmittance for pure PC and anthracene doping PC films for different doping ratio are shown in figure (5). It is obvious that behavior of the transmission spectrum of pure PC and anthracene doping PC films for different doping ratio of anthracene are opposite to that of the absorption spectra.

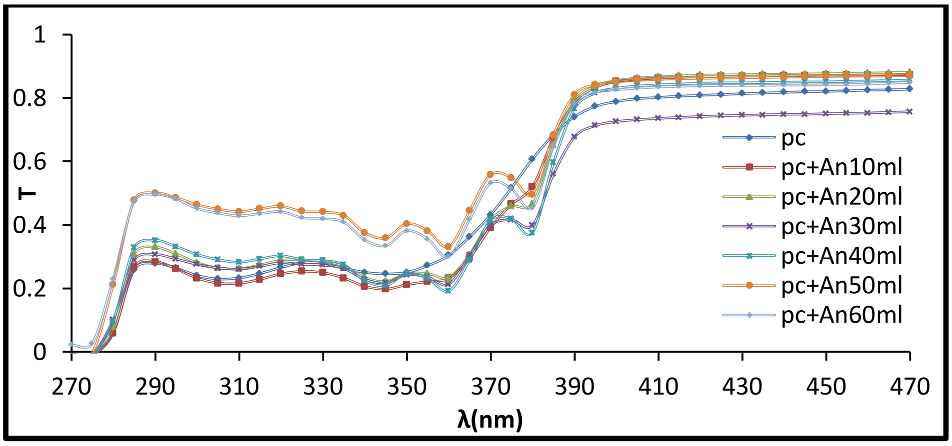

Figure (5) Transmission spectrum of pure PC and anthracene doping PC films in different doping ratio

3.5 Reflection Spectrum

Reflection spectrum is calculated from absorption and transmission spectrum according to equation (4). The reflection spectrum of pure PC and anthracene doping PC films for different doping ratio are shown in figure (6). Increase the doing ratio of anthracene lead to increase the reflection.

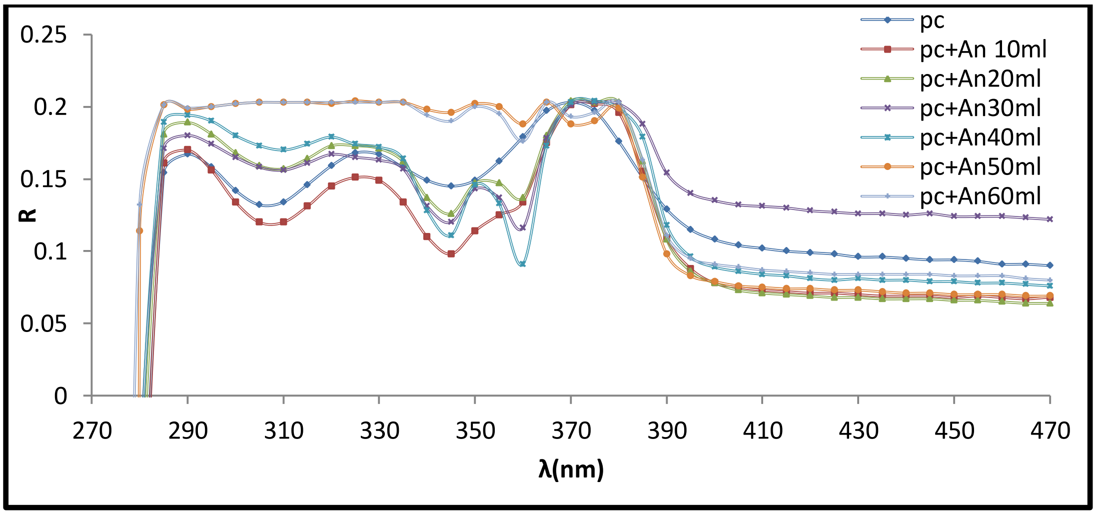

Figure (6) Reflection spectrum of pure PC and anthracene doping PC for different doping ratio

3.6 Absorption Coefficient

The absorption coefficient is calculated from equation (2) for all samples. The absorption coefficient of pure PC and anthracene doping PC films for different doping ratio are shown in figure (7). The absorption coefficient used to conclude the nature of electronic transition. When the values of absorption coefficient are high ($\alpha > 10^4 cm^{-1}$) at higher energies, you will expect direct electronic transition and the energy and momentum conservation for the electron and photon. Whereas when the values of absorption coefficients are low ($\alpha < 10^4 cm^{-1}$) at low energies, indirect electronic transitions have been expected and energy and momentum preserve of electron and photon by phonon help [16]. In our result, the value of absorption coefficient for all samples less than 10^4 cm^{-1}, so that the indirect electronic transition will deduced.

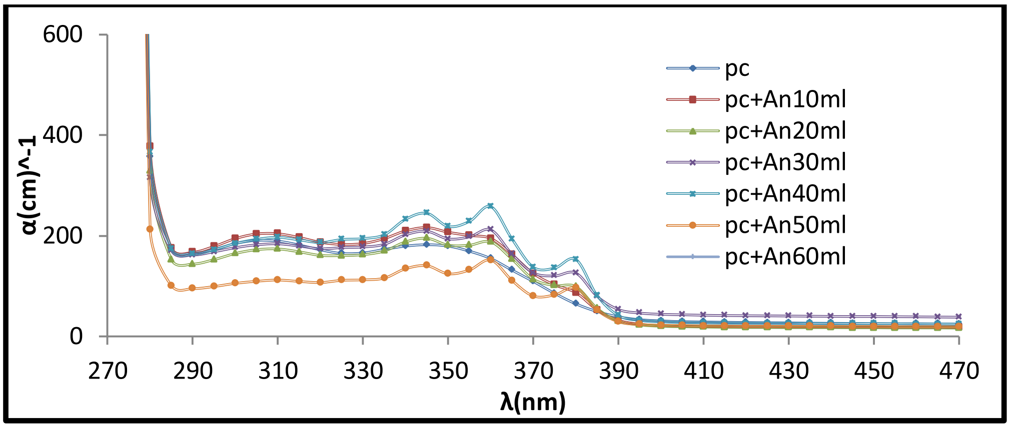

Figure (7) Absorption coefficient of pure PC and anthracene doping PC films for different doping ratio

3.7 Optical Energy Gap

The energy gap (E_g) can be find by plotting (α h ν) $^{1/r}$ versus (hν) in range of the high absorption followed by extrapolating the linear region of the plots to (α h ν) =0[17]. From the value of absorption coefficient of pure PC and anthracene doping PC films, indirect transition will happened at r=2. The energy gap of pure PC can be measure from the figure (8) and it is equal to (4.42 eV) this is agree with result obtained by H. M. Ghanem et al [11] and N. J. Hameed [12]. The energy gap of anthracene solution calculated from figure (9) and equal to (4.69eV). When anthracene added to PC polymer with different doping ratio, the energy gap was calculated from figure (10) and slight change will be observed. The energy gap for all films listed in the table (1).

Table (1) Energy gap of anthracene doped polymer polycarbonate films for different ratio.

Doping ratio of anthracene(ml)	PC	10ml	20ml	30ml	40ml	50ml	60ml
E_g (eV)	4.42	4.42	4.43	4.43	4.43	4.44	4.39

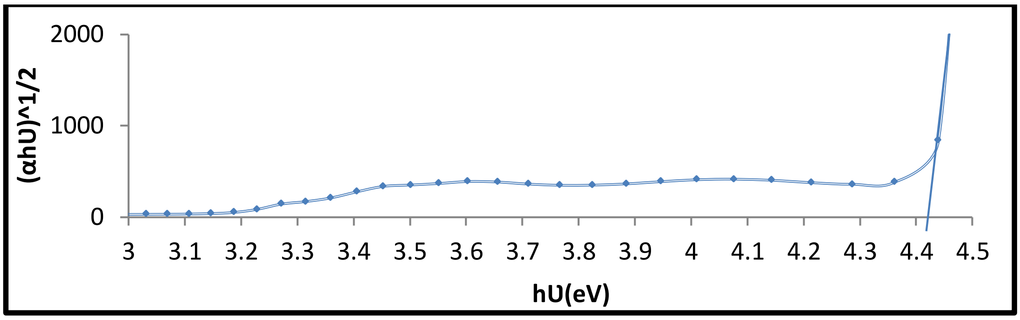

Figure (8) Optical energy gap of polycarbonate (PC)

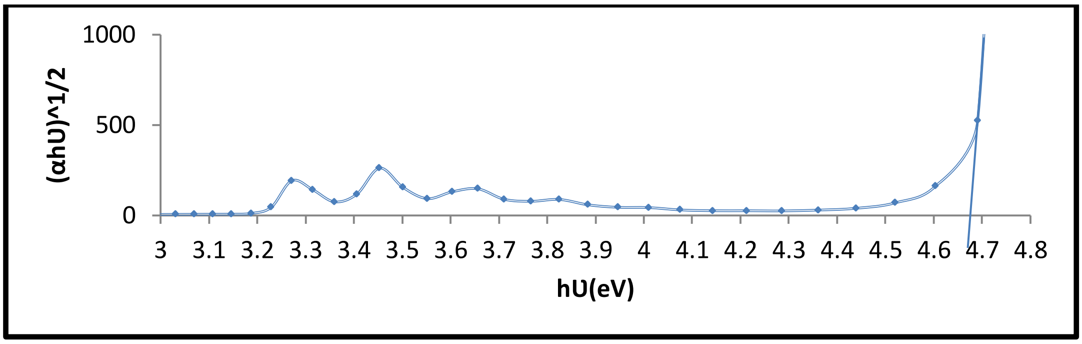

Figure (9) Optical energy gap of anthracene

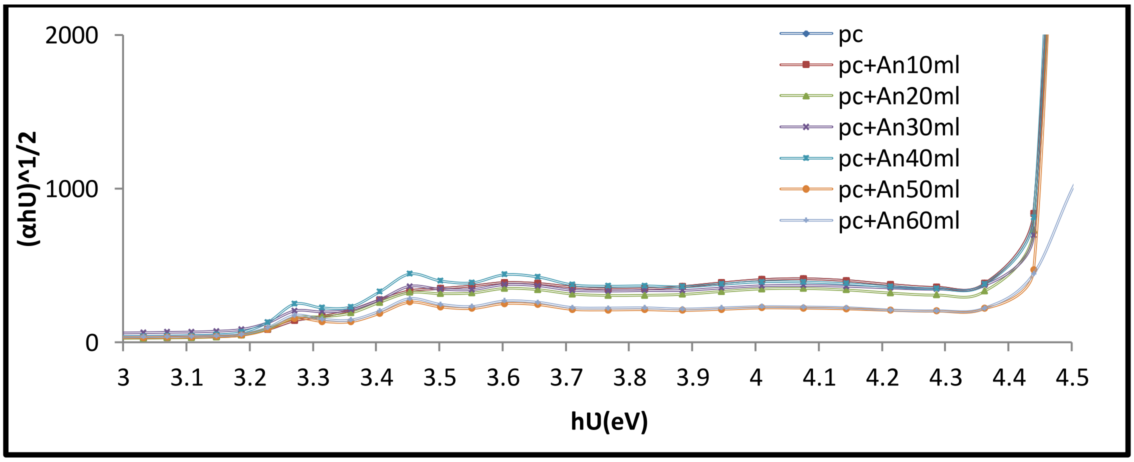

Figure (10) Optical energy gap of anthracene doping PC films for different doping ratio

3.8 Refractive Index

The refractive index is an important parameter. The refractive index of pure PC and anthracene doping PC films for different doping ratio are shown in the figure (11). The refractive index increased with increase the doping ratio.

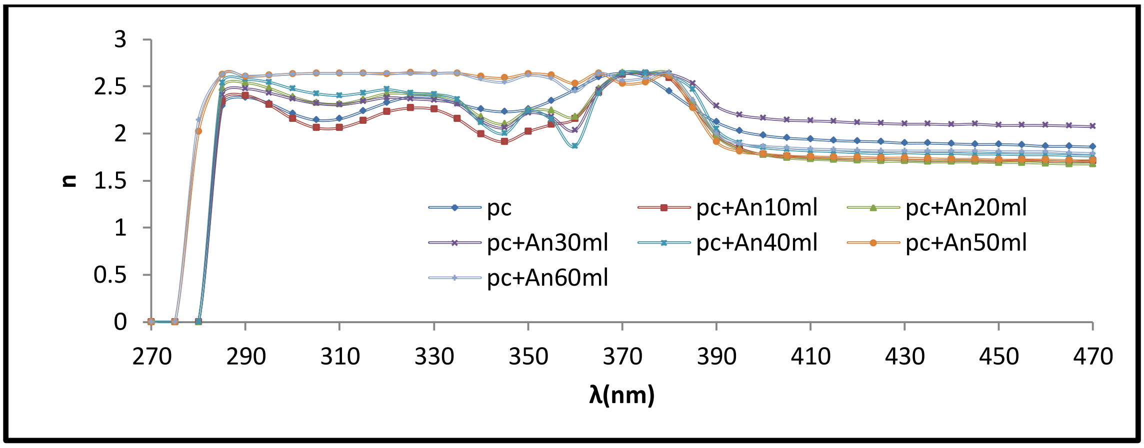

Figure (11) Refractive index of pure PC and anthracene doping PC films for different doping ratio

3.9 Extinction Coefficient

The extinction coefficient depended on absorbance and can be calculated by equation (3). The extinction coefficient of pure PC and anthracene doping PC films for different doping ratio are shown in the figure (12). The extinction coefficient increases with increase doping ratio till (40ml) then the extinction coefficient decrease.

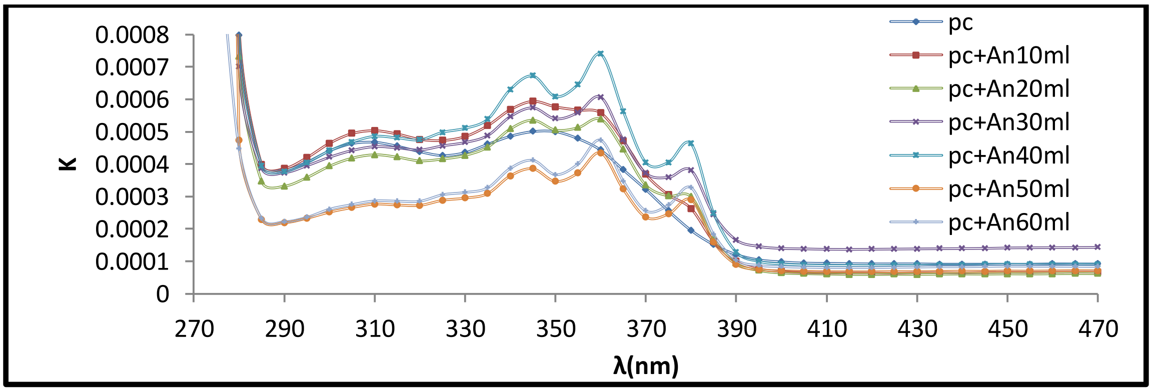

Figure (12) Extinction coefficient of pure PC and anthracene doping PC films for different doping ratio

3.10 Dielectric Constants

Optical constant are very useful for the quantitative determination of the electronic band structure of solid from information of optical reflectivity, transmission and refraction provide the way to determine the dielectric constants of solid, which is related to the band structure. The real and imaginary parts of dielectric constants can be calculated by using equations (8) and (9) respectively. The real part of dielectric constant of pure PC and anthracene doping PC films in different doping ratio are shown in figure (13). The real part of dielectric constant increase with increasing doping ratio. Imaginary part of dielectric constant of pure PC and anthracene doping PC films in different doping ratio are shown in the figure (14).

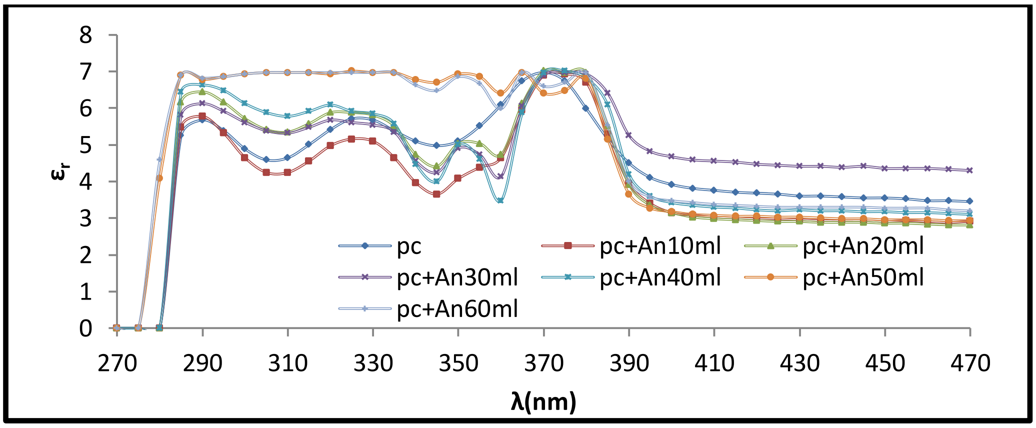

Figure (13) Real part of dielectric constant for Pure PC film and anthracene doping PC films for different doping ratio

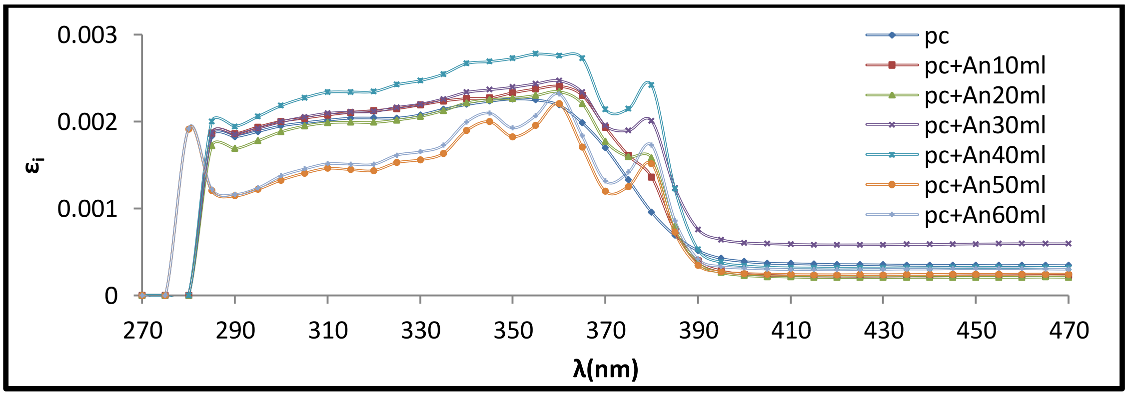

Figure (14) Imaginary part of dielectric constant for pure PC film and anthracene doping PC films for different doping ratio

4. Conclusions

From this study it can calculated that the addition of anthracene affected on optical properties of polycarbonate films as doping and prepared by cast method. The energy gap of PC is 4.42(eV) and doesn't effect by doping with anthracene, and the transition is indirect.

5. References

1- H. Jabur Ali,"The Electrical and Optical properties of Annealed Cd_2SnO_4Thin Films Prepared by Chemical Spray Pyrolysis Technique", M.Sc.Thesis, Physics Departement, College of Science, University of Al-Mustansiriyah, Baghdad, (2010).

2- E. Yousif and R. Haddad," Photo Degradation and Photo- Stabilization of Polymers, Especially Polystyrene: Review", Springer Open Journal, 1-32, 2:398, (2013).

3- R. Klein, "Laser Welding of Plastics", 1st Addition, Wiley-VCH Verlag GmbH & Co. KGaA, (2011).

4- M. Raheem Fraih, "Study of Thermal Aging Effect on Optical Properties of Some Polymer Blends", M.Sc. Thesis, Department of Applied Sciences, University of Technology, (2010).

5- G. F. Tjandraatmadja, L.S Burn and M.J. Jollands, "The Effects of Ultraviolet Radiation on Polycarbonate Glazing", Institute for Research in Construction, National Research Council Canada, Ottawa ON,K1A 0R6,Canada, pp.884-898, (1999).

6- G. Streetman Banerjee, "Solid State Electronic Devices", the University of Texas at Austin, (2006).

7- M. Balkanski, "Optical Properties of Solids"Vol.2, Amsterdam, New York. Oxford (1992).

8- N. M. Sloomi, "Spectrophotometric Study of Gamma Irradiated polystyrene Composites", M.Sc. Thesis, University of Mustansiriyah, College of Science , Physics Department, (2016).

9- J. Ballato, and S. Foulger, "Optical Properties of Perfluorocyclobutyl Polymers", J. Opt. Soc. Am. B, 20(9), 1838-1843, (2003).

10- J. Tauc, A. Menth, and D. Wood, "Optical and Magnetic Investigation of the Localized States in Semiconducting Glasses", Phys. Rev. Lett., 25, 749, (1970).

11- H. M. El Ghanem, S. A. Saqa'n, M. Al Saadi and S. M. Abdul Jawad,"On the Electrical and Optical Properties of Polycarbonate/$MnCl_2$Composite", Journal of Modern Physics, 2, 1553-1559, (2011).

12- N. J. Hameed & M. R. Fraih, "Study of the Optical Constants of the PMMA/PC Blends", Eng. & Tech. Journal, 29(4), 698-708, (2011).

13- F. J. Kadhum, "Optical Properties of Laser Dye Rhodamine B Doped Polymethylmethacrylate – Polycarbonate Films", Journal of College of Education, no(3), (2016).

14- J. Kunnil, S. Sarasanandarajah, E. Chacko, and L. Reinisch**,** "Fluorescence Quantum Efficiency of Dry Bacillus GlobigiiSpores"**,** Optics Express**,** 13(22), 8969-8979, (2005).

15- S. Gupta, D. Choudhary, A. Sarma, "Application of Excitation-Emission Fluorescence Matrices and UV/Vis Absorption to Monitoring the Photo catalytic Degradation of Commercial Humic Acid". J, Polym. Sci. Part B: Polymer Physics, 38, 1589-1594, (2000).

16- F. L. Rashid, A. Hashim, H. Ahmed, "Preparation of (PS-PMMA) Copolymer and Study the Effect of Sodium Fluoride on its Optical Properties", Chemistry and Material Research, 3(7), 55-58, (2013).

17- T. J. Alwan, "Refractive Index Dispersion Optical Properties of Dye Doped Polystyrene Films" Malaysian Polymer Journal, 5(2), 204-213, (2010).