International Journal of Scientific Engineering and Applied Science (IJSEAS) – Volume-2, Issue-5,May 2016
ISSN: 2395-3470
www.ijseas.com

Study of the optical properties for 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol extraction from eggplants peel

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Abstract

The optical properties for 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol have been studied in the range of wave length (300-900)nm. The absorption (A), transmittance (T), the absorption coefficient (α), refractive index (n), extinction coefficient (k), real dielectric constant (ε_r) and imaginary dielectric constant (ε_i) have been all investigated. The direct energy gap ($E_g^{dir.}$) and Urbach tail (E_u) have been calculated, they are (2.8, 0.9) eV respectively.

Keyword: Optical properties, 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol, eggplants peel.

1. Introduction

The optical properties are very important in the field of optics applications such as integrated optics, optical information, optical modulation and optical data, the optical properties of materials change or affect the characteristics of light basing throw it [1].

Three beneficial optical properties, refractive index, absorption coefficient and extinction coefficient which are generally called optical constants, they are determined from optical behavior of the material [2].

One of the different methods used to deposited thin films is the spray pyrolysis deposition technique, gaining traction in the scientific community because of its cost effectiveness and ease. Spray pyrolysis has been applied to deposit a wide variety of thin films. These films were used in various devices such as solar cells, sensors and sold oxide fuel cell [3,4].

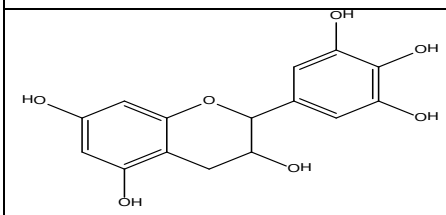
There has been increasing realization in recent years that several plant derived polyphenolic compounds, one of these compounds is 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol extraction from eggplant peel [5], in this papers we study the optical properties of it.

2. Experimental details

2.1. Extraction of the pigment

100 gm of eggplants peel have been collected and washed by the distillation water, dried at 50^0C for 72 hours and grinding, and dissolved in 100ml of methyl alcohol. The solvent was left in 15^0C for 24 hours, then filtered with filter paper. 0.02 gm of yellow powder was produced [6]. Table (1) shows the chemical structure and some of the physical properties of the pigment.

Table (1):Chemical structure and physical properties

Chemical structure	Physical state	M.P (°C)	Color	M.W	Density g/cm^3
	powder	>153*	yellow	306.27	1.6

2.2Preparation of Thin Film

(0.01 mol. 0.01gm) of 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol pigment dissolved in 25 ml of dimethyl sulfoxide (DMSO). The solvent heated up to 60 ^{0}C and have been stirred for 45 min, and it left while the heat reached to room temperature, then the solution was filtered. The 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol thin film have been deposited on the clean glass substrate of dimensions of (2.7, 2.5) cm, by repeat-spry method. The nitrogen gas have been used to produce the 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol thin film, the thickness of the thin film have been calculated by using the equation below [7].

$$\mathbf{d= m_2 – m_1/ \rho a} \quad \mathbf{(1)}$$

Where d: thickness, m_1: the mass of glass substrate, m_2: the mass of glass substrate and the 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol thin film, ρ: the density of Pheomelanine and a: the area of thin film. The thin film thickness was 14* 10^{-5} cm.

3. Results and Discussion

3.1 Infrared spectrum

The dye powder was identified by IR spectroscopy in the range (4000–400) cm^{-1} as shown in Figure (1).

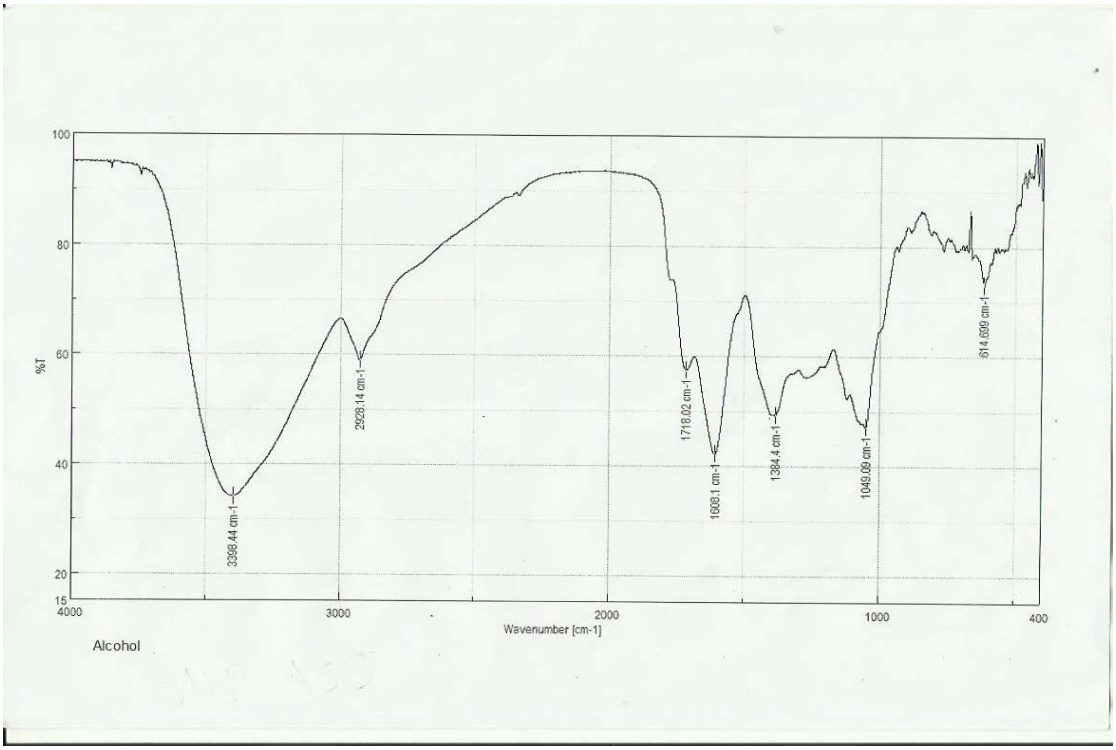


Figure (1): IR-spectrum of 2-(3,4,5-trihydroxyphenyl)chroman-3,5,7-triol

The stretching vibration of the OH group appeared in the region of (3398) cm^{-1}. The band shows broad appearance due to its relatively low frequency. It can be concluded that the (-OH) group may form a hydrogen bonding. The (-C=C-) stretching vibration of the aromatic ring is cited at (1608) cm^{-1}. Stretching vibration of the (-C-H) aromatic appears at (2928) cm^{-1}. The all mentioned bands are given in Table 1.

Table (2): Major IR absorption bands (cm^{-1}) of 2-(3,4,5-trihydroxyphenyl)chroman-3,5,7-triol .

Functional group	OH	C=C aromatic	C-H aromatic
ν(cm^{-1})	3398	1608	2928

3.2. The Optical Properties

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 (CE-7200) at room temperature. The curves of the absorption and transmittance of the thin film is shown in fig. (2), the high value of

spectra of thin film appeared at (300) nm, which represents the transition (π-π^*) founds in (-c=c-) bond,

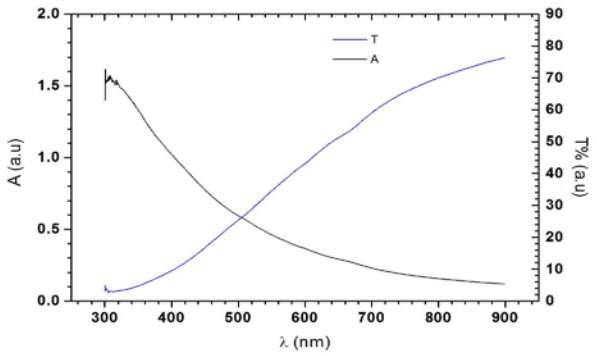


Figure (2): The absorption and transmittance spectra of thin film.

The absorption coefficient has been determined from the relation (α= 2.303 A / d) [9].The extinction coefficient (k) is related to the absorption coefficient (α) by the relation ($k = \alpha\lambda/4\pi$) where π is 3.14 [10]. The refractive index (n) has been calculated by the equation (2) [11].

$$\mathbf{n} = \left(\frac{1+R}{1-R}\right) + \sqrt{\left(\frac{4R}{(1-R)^2} - K^2\right)} \quad \textbf{(2)}$$

Figure (3) shows the behavior of the absorption coefficient (α) with the energy of incident photons (hν), leading to the transitions between electron bands are directly ($\alpha > 10^4$ cm^{-1}) [12].

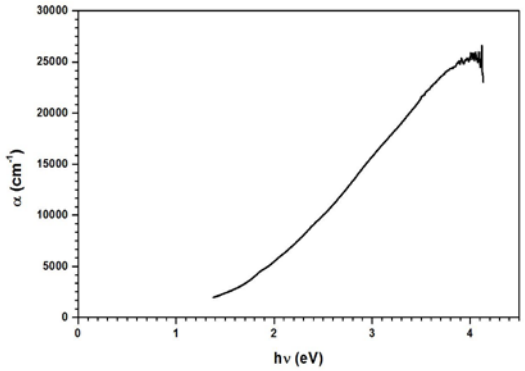


Figure (3): The absorption coefficient of thin film.

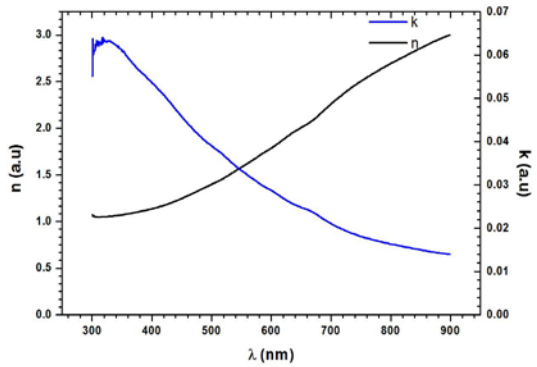


Figure (4): The extinction coefficient and refractive index of thin film.

The extinction coefficient (k) and refractive index (n) are shown in Figure (4). The highest values of extinction coefficient (k) can be seen in UV region, showing that the prepared film is highly transparent. This discretion reverse for the refractive index (n) has been the highest values of its located near IR region, in which the refractive index (n) is a key parameter for the device design. A very important and interesting relation between optical and dielectric properties is $n^* = n - ik = (\varepsilon)^{1/2} = (\varepsilon_r + \varepsilon_i)^{1/2}$, where n^*, ε, ε_r, ε_i, are the complex refractive index, complex, real and imaginary dielectric

constants respectively. Therefor $\varepsilon_r = n^2 - k^2$ and $\varepsilon_i = 2nk$ [13]. They are draw as function to exited photon energy in Figure (5).

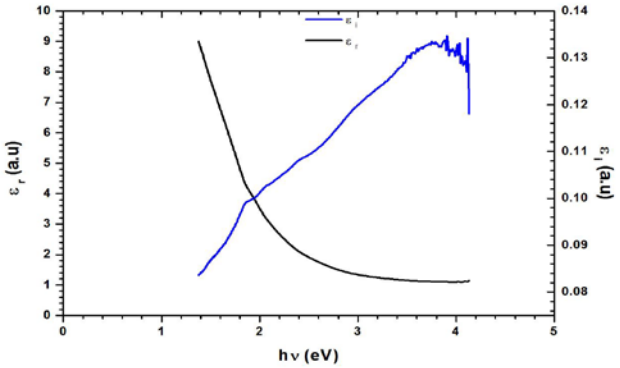


Figure (5): The real and imaginary parts of dielectric constant as a function of incident photon energy.

It is noted that the real dielectric constant decreases with increasing of photon energy, while the imaginary dielectric constant decreasing. This behavior corresponds to the behavior of refractive index and extinction coefficient. The optical energy gap can be determined from the analysis of the absorption coefficient (α) by using the following expression.

$$\alpha h\nu = B (h\nu - E_g^{opt.})^r \quad (3)$$

where B is constant (independent of photon energy) for respective transitions , E_g^{opt} is optical energy gap and r equal to 1/2 for direct allowed transition and 2 for direct forbidden transition ($\alpha > 10^4$ cm^{-1}) [14]. Figure (6) shows the allowed direct transition, plotting $(\alpha h\nu)^2$ against incident photon energy ($h\nu$), the energy gap is determined from the intercept on the axis of incident photon energy of the liner fit of the larger energy of photons. The direct energy gap has been 2.8 eV.

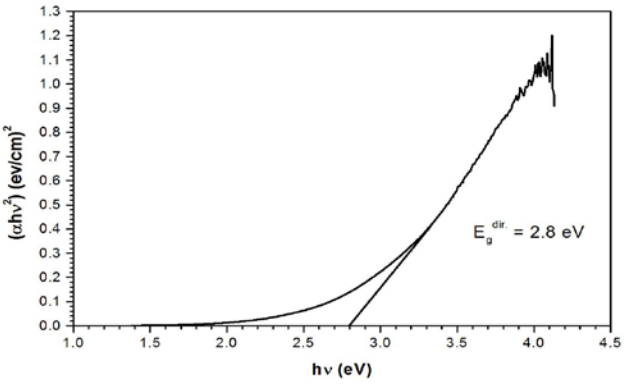


Figure (6): The plots $(\alpha h\nu)^2$ vs. photon energy hν for 2-(3,4,5-trihydroxyphenyl)chroman-3,5,7-triol thin film.

The chemical disorder in materials is called Urbach tails or energy where the molecules have big molecular weight like pigments and polymers, for example, and it is given by using equation (4).

$Ln(\alpha) = C + h\nu / E_u$ (4)

Were C is constant and E_u represents Urbach tail [15,16], calculated by taking inverse of the slope of the [illegible].9 eV.

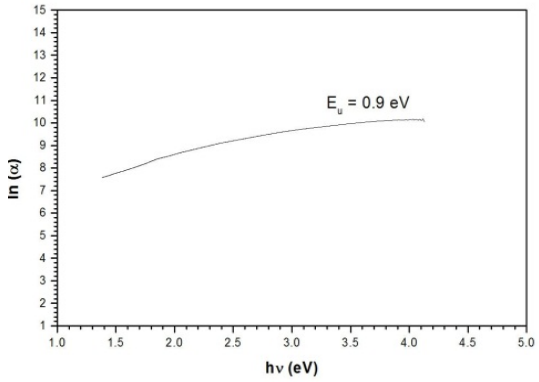


Figure (7): Urbach tail for2-(3,4,5-trihydroxyphenyl) chroman-3,5,7-triol thin film.

Conclusions

In this research, the maximum value of absorbance has benn found in the UV region. The absorption coefficient (α) increases with increasing incident photon energy and order of it is 10^4 cm^{-1}, therefor the transitions between the bands of energy are direct. The refractive index (n) increases with increasing wave length, but the extinction coefficient (k) decreases. The direct energy gap and Urbach tails are calculated and the magnitudes of them are 2.8, 0.9 eV, respectively. It means that the 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol pigment has high disorder in chemical structure and semiconductor characteristics as well as having wide of extended levels between valance and conduction bands.

Table (3) Some of the optical constants for the 2-(3,4,5-tri hydroxyl phenyl) chroman-3,5,7-triol pigments

λ (nm)	**442.6**
n (a.u)	**1.2**
k (a.u)	**$470.16 * 10^{-4}$**
α (cm^{-1})	**$1.3342 * 10^4$**
ε_r (a.u)	**1.5**
ε_i (a.u)	**0.11**
$E_g^{dir.}$ (eV)	**2.8**
E_u (eV)	**0.9**

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International Journal of Scientific Engineering and Applied Science (IJSEAS) – Volume-2, Issue-5,May 2016
ISSN: 2395-3470
www.ijseas.com

دراسة الخواص البصرية لـ 2-(3،4،5- ثلاثي هيدروكسيل فنيل) كرومين -3،5،7- ترايول المستخلصة من قشور البذنجان

نورس محمد احمد [2] ، وسام عبدالحسن راضي[2]، عبدالجبار عبدالرضا جابر[1]* محمد توفيق عبيد
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الخلاصة
تم في هذا البحث استخلاص صبغة 2-(3،4،5- ثلاثي هيدروكسيل فنيل) كرومين -3،5،7- ترايول من قشور البذنجان. وقد درست الخواص البصرية لها كالامتصاصيه والنفاذيه ومعاملات الامتصاص والانكسار والخمود وثابت العزل الحقيقي والخيالي، كما حسبت فجوة الطاقة وطاقة اورباخ حيث كانت القيم (0.9, 2.8) الكترون فولت على التوالي.

الكلمات المفتاحية: الخواص البصرية، 2 -(3،4،5- ثلاثي هيدروكسيل فنيل) كرومين -3،5،7- ترايول، قشور البذنجان