

The Extraction of Alcea Rosea Organic Dye and Its Characterization of Optical Properties

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ABSTRACT: In the present study, the optical properties of a natural dye extracted from Alcea rosea flowers were investigated. The color extraction procedure was performed using a nontoxic solvent ethanol to enhance human safety and the ecological framework. Fourier transform infrared spectroscopy was employed to determine the functional groups of the natural dye obtained from Alcea rosea flowers. The optical properties of dye were achieved by the directed thin film using UV-Vis spectroscopy and analyzed absorption spectra, coefficients, refractive indices, extinction coefficients, and optical energy bandgap. A broad absorption band occurs over an extensive waveband with peak at 380 nm. The occurrence of a low indirect bandgap in a thin film was discerned at 3.9 eV, with Urbach energy noticed in a state of 0.23 eV.

Keywords: Green materials, Thin film, Optical properties, Natural dye, Biomaterials

INTRODUCTION

Natural dyes derived from plants are biomaterial and have a negligible effect on the environment. For centuries, these natural products have been the focus of human efforts, including coloring textiles, enriching artworks, and even food. Recently, the interest in these dyes has increased significantly. Among the numerous natural dye sources available, Alcea rosea, belongs to the Malvaceae family, and has demonstrated great promise in several applications. The renewed interest in hollyhock can be attributed to its high pigment content and has the potential to extract dyes with exceptional optical properties [1-5]. The flowers and leaves identify with a riot of color and has a medical and textile applications for a for a long time until the current time. The dye extracted from this plant discloses intriguing compounds because the petals and leaves of hollyhock contain a diverse combination of pigments. The dye extracted from the most plants has chemical components containing many pigments. The chemical separation processes for the pigments present in the Alcea rosea flower yields to different colors, ranging from deep purple to soft pink. The appropriate use of the

pigment depends on several factors, including: its color degradation, stability, absorption, and reflectance spectra. [8, 9]. Studying the spectral properties of a substance is important in the issue of light-matter interaction that serves in optical applications, as solar cells, LEDs, and sensors [10-12]. The availability of green materials, such as plant pigment, represents an opportunity that is easy to implement in applications of optoelectronics. Analyzing the physical structure of a pigment through the absorbance determines its versatile, sensitive, and quantitative and hence its suitability in an application.

This study focuses on identifying the optical properties of the Alcea Rosea dye, pointing to enhance the field of organic optoelectronics. As various analytical approaches, findings, and discussions are studied, a desired future emerges. It involves the possible usage of natural dyes like Alcea Rosea to encourage the development of ecologically friendly organic semiconductor optoelectronic technology. The Alcea Rosea dye inspires further research into the fusion of traditional practices, environmental concerns, and technological advancements.

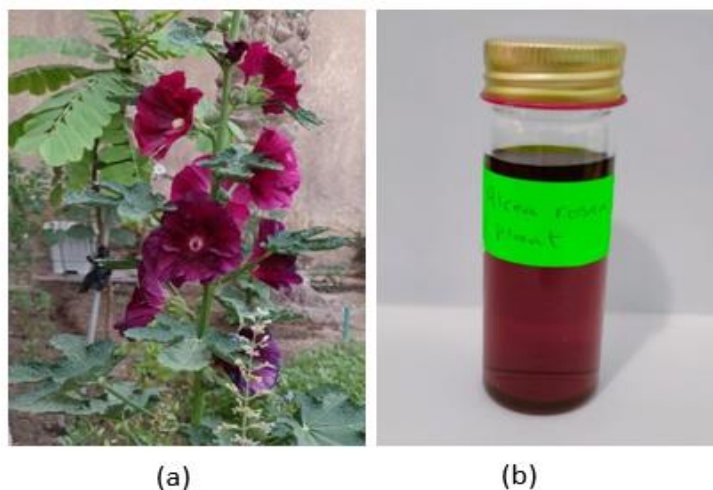


Figure 1: The Alcea rosea flower and its extracted colorant solution.

MATERIALS AND METHODS

Alcea rosea is a plant commonly used to create a crude dye extract and can be found in both private and public gardens in Basrah. The pigment extraction process from the Alcea rosea plant utilized a magnetic stirring apparatus (BOECO Hot Plate Magnetic Stirrer, model MSH 420) with a stirring capacity of up to 15 liters, adjustable stirring speeds ranging from 60 to 1110 rpm, and the ability to maintain an ambient heating temperature of up to 450°C. The FTIR spectra were recorded using the Shimadzu IR Prestige 21 instrument, including the 200 - 4000 cm^{-1} spectral band. The UV-Visible spectra, with wavelengths ranging from 200 to 1100 nm, were measured using the spectrophotometer (CE-7200), double beam.

Dye extraction protocol

The initial step preceding the extraction procedure involved gathering approximately 250 grams of flowers. The petals were carefully rinsed with distilled water to remove any traces of dust particles. Subsequently, the purified petals were left for 10 days at room temperature in a dark and dry storage area before being crushed into a powdery form. In a lidded glass beaker, 50 milliliters of distilled water were added to 0.05 g of the powdered substance. Filters made of medium-fast paper with a thickness of 0.33 mm and a weight of 55

g/m^2 were used for filtration, resulting in an aqueous extract specifically derived from the Alcea rosea flower. The powdered dye and water were combined in a ratio of 1:50. Magnetic stirring was set to 60°C for a duration of 60 minutes. The resulting solution or extract is shown in Figure 1(a), where liquid hues can be observed.

Preparation process of thin film

A suitable substrate, typically made of glass measuring 2.5x7.5 cm, is carefully selected and treated to ensure optimal adhesion. The treatment process involves thoroughly cleaning the substrate with a specialized solution and applying a thin layer of adhesive. The natural dye solution is meticulously applied to the treated substrate using spin-coating, ensuring precise and controlled application. The substrate is placed on a rotating platform and rotated at a speed of 1000 rpm, facilitating the even distribution of the dye. Following the application, the thin film undergoes a curing process in an electric oven set to 60°C for 25 minutes. The controlled heat exposure enhances the bonding between the dye and the substrate, ensuring a secure attachment. This method produces a sustainable and visually striking thin film with vibrant colors, making it suitable for a wide range of applications.



Investigation of the FTIR spectroscopy

The valuable analytical technique FTIR was employed to identify the functional groups and molecular structure of the compound, as depicted in Figure 3. Spectrum characterization involves the identification of different absorption bands which show how bonds in the molecule interact with electromagnetic waves within IR region. A broadband absorption located at 3326 cm^{-1} is clearly represented by the stretching of hydroxy groups (O-H). Two bands detected at 2936 cm^{-1} and 2890 cm^{-1} are attributed to symmetric and

asymmetric (C-H) bond stretching of the methylene group, respectively. A strong band peaked at 1729 cm^{-1} is assigned to stretching vibration of the ketone carbonyl group (C=O). Other absorption bands include band at 1631 cm^{-1} related to double bonds (C=C) stretching within aromatic ring, band at 1180 cm^{-1} assigned to (C-O) bond stretching of ether group and band at 1069 cm^{-1} because of (C-O) bond stretching of the alkoxy group. The obtained results are in good agreement with earlier research [13].

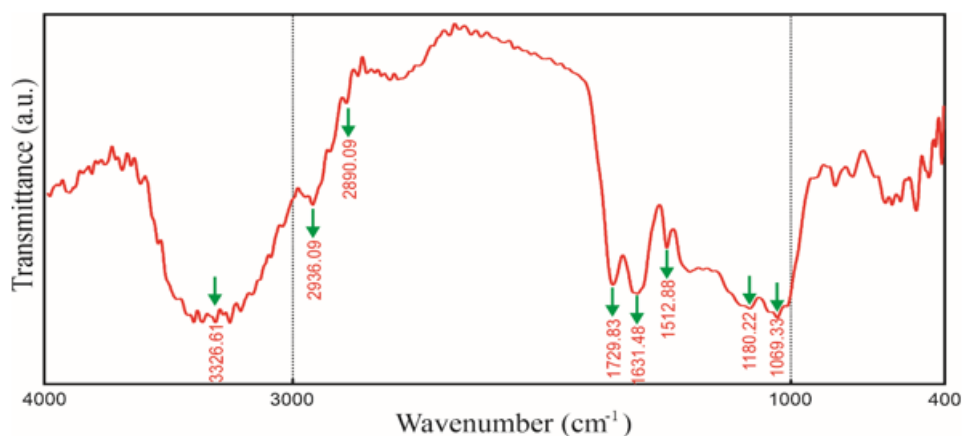


Figure 3: The FT-IR spectroscopy of Alcea rosea powder at room temperature.

RESULT AND DISCUSSIONS

The extracted dye shows strong absorption in the vicinity of the 380 nm wavelength. Anthocyanins, an essential chemical component of dyes, contribute to the red color found in various plants. These pigments possess a broad absorption peak spanning from the ultraviolet to the near-visible

spectrum. In the field of photovoltaics, dye compounds demonstrate a remarkable feature: a broad absorption peak spanning from 400 to 650 nm, resulting from HOMO-LUMO charge transfer transitions. Additionally, the extracted aqueous dye displays a purple color.

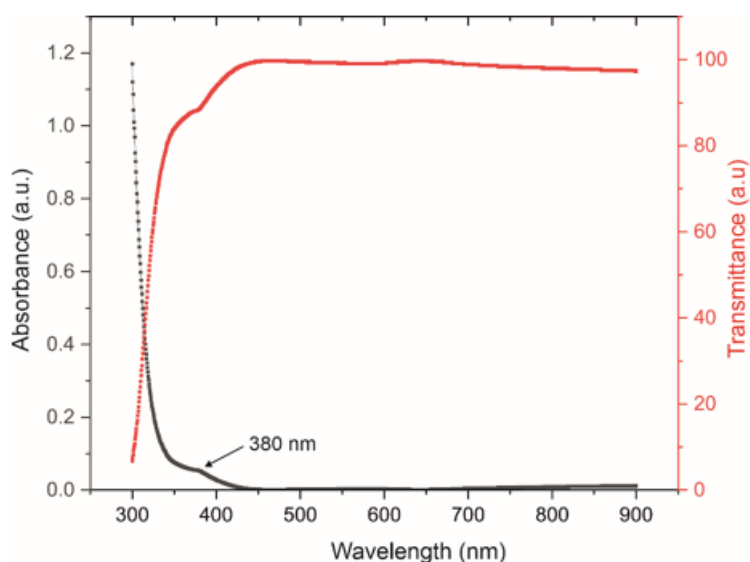


Figure 4: Optical absorption (black curve) and transmittance (red curve) spectra of Alcea rosea thin film.

Additionally, the spectra in figure 4 show that the portulaca grandiflora dye exhibits minimal variations in its absorption properties across the visible wavelength region, despite its low absorption at the peak. Absorption peaks ranging from 300 to 435 nm are typically associated with the excitation of $n \rightarrow \pi^*$ transitions due to their low energy requirements. This phenomenon, referred to as the R-band, occurs within a molecule due to the presence of unsaturated chemical groups, which are often indicated by chromophore groups.

Optical absorption coefficient and Optical energy gap.

To determine the kind of electronic transfer that takes place within substance's electronic structure, the absorption coefficient plays a crucial role, particularly within the absorption region [14]. The equation below was used to get the absorption coefficient:

$$\alpha = \frac{1}{d} \ln \ln \left[\frac{(1-R)^2}{2T} + \sqrt{\frac{(1-R)^4}{4T^2} + R^2} \right]$$

(1)

R and T represent the reflection and transmittance indices, respectively. The film thickness is denoted as 'd' and its value of 234 nm This parameter is calculated using the conventional method, which takes into consideration the masses of both the substrate of glass (m_1) and the coating dye on same substrate (m_2), as explained:

$$d = \frac{m_2 - m_1}{\rho a}$$

(2)

The absorption coefficient of the natural dye under investigation is illustrated in Figure 5(a), with ρ representing the density of the dye and a denoting a specific sample area. The spectra exhibit a prominent absorption band in the 300-450 nm region, which is caused by electronic transitions ($n \rightarrow \pi^*$) of compounds/components in the dye. The absorption coefficient is often used to calculate the energy band gap. The HOMO-LUMO gap is considered an important physical characteristic controlling semiconductor and dielectric properties. The optical gap is used to describe the formation of a free electron state that is isolated, uncorrelated, and weakly energetic. In solids, the migration of particles is connected to the energy gap effect. In this study, the determination of energy gap values involves calculating intercepts on the x-axis between $(\alpha h\nu)^2$ and $h\nu$, which represent specific parameters.

Tauc's relationship, as given in Equation 3 below, is used to explain the analytical approach used in this study [15]. This relationship provides insight into the calculation of energy gap values and their relationship to $(\alpha h\nu)^2$ and $h\nu$:

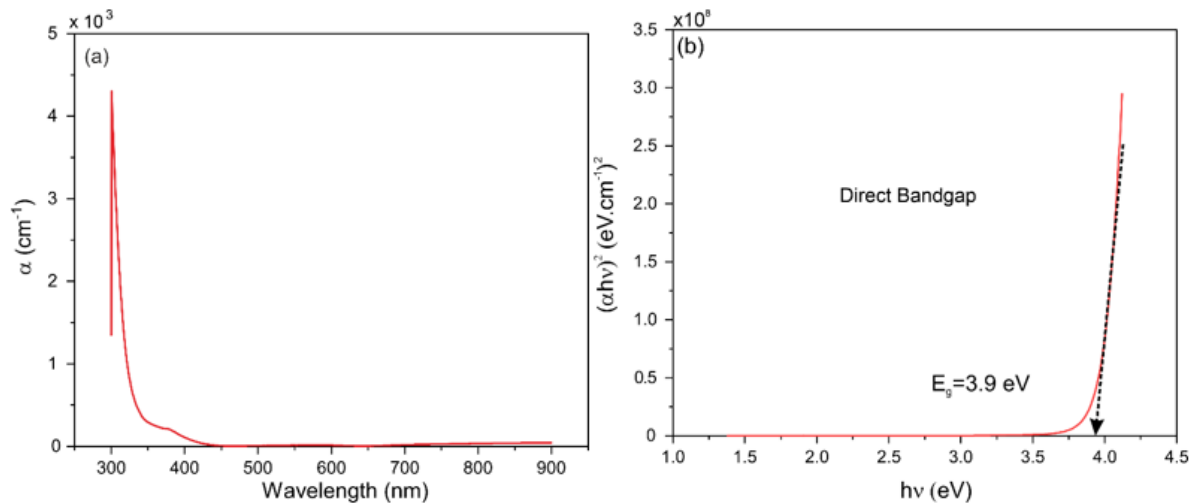


Figure 5: (a) Absorption coefficient of thin film, and (b) direct bandgap calculation using Tauc relation.

$$\alpha = \frac{A\{(h\nu - E_g)\}^\gamma}{h\nu}$$

(3)

A is a constant that depends on the transition probability, whereas γ indicates the index of the density of states distribution, which changes depending on the specific transition method (direct or indirect). Figure 5(b) depicts the plot of $(\alpha h\nu)^{1/2}$ versus $h\nu$ for the Alcea rosea sample. The energy value of samples deposited at normal temperature is

approximately 3.9 eV. New localized atomic energy levels have emerged below the conduction band in the electronic structure of the dye. These defective bands cause the creation of localized tail states that are highly efficient at electron collection within the "Urbach region," encompassing both the valence and conduction band levels. The Urbach energy of the system is closely associated with its structural perturbation function [16, 17]. An increase in Urbach energy corresponds to an increase in disorder due to amorphous

structures or insufficient crystallinity. The calculated Urbach energy for the thin layer of Alecea rosea is 0.23 eV, as shown in Figure 6. The material changes might be caused by internal

fields that affect how chemical groups interact or by a reduced ability to convert weak connections into defects.

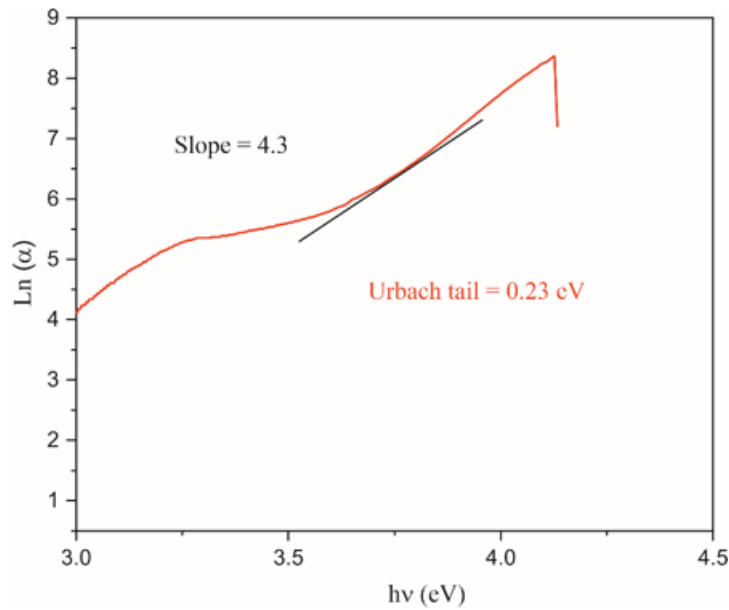


Figure 6: Urbach energy calculation via the graphical slope ns. Ln α

Refractive index and Extinction coefficient

Important factors for determining the optical properties of a sample include the extinction coefficient and refractive index. In the study of dyes or compounds, the optical parameters, represented by n and k , measure a material's capacity to absorb light at a certain wavelength. These parameters can be incorporated into a complex frequency-dependent equation, with the imaginary part k and the real part n . It is well known

that the n and k parameters can be obtained by using the relations provided in equations (4 and 5) [18]:

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

(4)

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

(5)

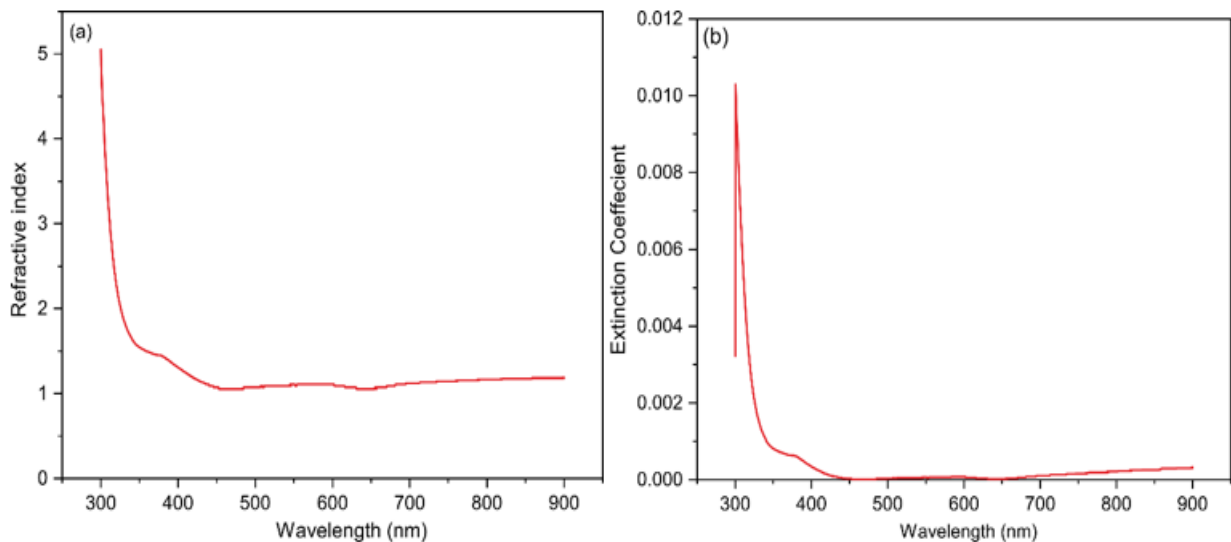


Figure 7: (a) Refractive index, and (b) extinction coefficient of Alcea rosea thin film.

The wavelength-dependent variation in the refractive index for the natural dye is depicted in Figure 7(a). A close inspection of the figure reveals that the refractive index for the organic dye consistently remains at approximately 2.5. Notably, there is a significant shift from this value in the visible region. The higher values of 'n' in the high-energy range can be attributed to its effect on light absorption beyond 300 nm. Figure 7(b) presents the calculated extinction coefficient, *k*, for the thin-film of portulaca grandiflora dye. The extinction coefficient, as is widely known, describes how a material interacts with light and its optical characteristics. Interestingly, the increase in the extinction coefficient value with wavelength in the case of the natural dye can be attributed to the scattering mechanism.

CONCLUSION

In conclusion, the results of this study demonstrate the potential for economically extracting dye from *Portulaca grandiflora* using a magnetic stirrer and water bath extraction technique. Absorption coefficient predictions, based on the study results, indicate an indirect bandgap energy of 3.9 eV and an Urbach energy of 0.23 eV. Additionally, the FTIR data profile reveals distinctive functional groups and provides an explanation for the influence of the solvent on the extraction of natural dyes. This work significantly contributes to our understanding of the optical properties of organic dyes, which is vital for optimizing their optoelectronic features.

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