Materials Science Forum
ISSN: 1662-9752, Vol. 1065, pp 13-21

Submitted: 2022-01-31
Revised: 2022-03-28
Accepted: 2022-03-28
Online: 2022-06-30

Effect of Static Magnetic Field on *Anchusa-Italica*- Doped Pentacene

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Keywords: Natural dyes, Pentacene, static magnetic field, Optical properties.

Abstract: This work is devoted to the influence of magnetized water on dye extracted from *Anchusa Italica* plant and doped pentacene thin films. The findings resulted in optoelectronic behavior, showing that using magnetized water in the extraction process gives rise to distinct and superior characteristics as compared to using regular water. The Fourier-transform infrared method was used to analyze the structural properties of an *Anchusa Italica*-doped pentacene thin film. A comparative study on two samples was carried out: the first sample was affected by a static magnetic field and the other one was not. Optical properties including the absorption spectra absorption coefficient, optical energy gap, conventional and refractive factors were investigated by applying ultraviolet-visible spectroscopy ranging from 300 to 900 nm. The estimated band gap edge of the dye/doped pentacene affected with magnetization was reduced from 2.61 to 1.76 eV and converted into the recommended direct band gap to contribute to optical systems. The absorption spectra of the sample with magnetization effect appears to be more efficient than the one extracted using regular water. The power transmission coefficients (indirect to direct) were also affected because of the magnetic extraction procedure. The complex refractive index was used to study the magnetization effect on the resonance mode and transparent indicator. The absorption index was enhanced to 570 nm in the spectrum, whereas there was also a low attenuation coefficient. This is the first time that magnetized sol has been used in dye extraction processes.

Introduction

A dye-doped polymer interface can produce a thin functional layer with a large and appropriate bandgap. This important combination (dye/polymer) provides a broad range of absorption by increasing electronic interaction between the dye electrolyte and the semiconducting electrode [1–5]. In combination, these features can enhance the efficiency of the energy conversion of optoelectronic systems. The natural dye serves as the prototype, while the polymer behaves as the electron-acceptor agent [6–9]. In consequence, attempts to exploit natural dyes/pigments as semiconductors were developed by improving the electron injection capacity between the valence and conduction bands [10–13].

The main advantage of dyes is that production can be achieved by purified water. One of the most important effects on extraction is magnetization due to control of the electronic structure, which leads to optimization of the optoelectronic characteristics. Several investigations have demonstrated that when water is subjected to a magnetic field, changes occur in its optical and physical characteristics [14–17]. Subsequently, a great number of theoretical studies based on quantum theory concepts were dedicated to investigating the role of the magnetization on physical and chemical properties [18–20]. The latter can be adjusted by exposing the produced laboratory solution to a magnetic field with a flux density extending between 0.1 and 0.8 T [21–23]. The liquid can be magnetized without the need for any extra energy by employing a permanent magnet. As an example, for a single water molecule, the essential characteristic is the magnetic field's potential to decrease intra-cluster hydrogen bonds, resulting in the large clusters being broken up into minutest and powerful inter-cluster hydrogen interactions. The magnetic field action also breaks the van der Waals molecules in water, as indicated in [24]. Magnetization of water may lead to enhance the efficiency of extraction process because of

the development of the viscosity and tiny aggregates of water molecules. This modification allows for higher absorption by the plant and rapidly penetration into cell membranes, respectively.
Given these reasons, the purpose of this work is to analyze and report on the extracted dye affected by a static magnetic field and its effect on the electronic properties when it is doped with one of the polymers. This study is a continuation of what was previously reported concerning the magnetic field effect on dye only [25]. For this purpose, the optical characteristics of *Anchusa Italica*-doped pentacene (*A. Italica*-doped PEN) thin films were examined by evaluating the effect of the magnetic field. To highlight this latter effect, a comparison between two different samples (ADP and MADP) was performed. To achieve this objective, two magnets were utilized to verify that the target under investigation was effectively subjected to a magnetized region.

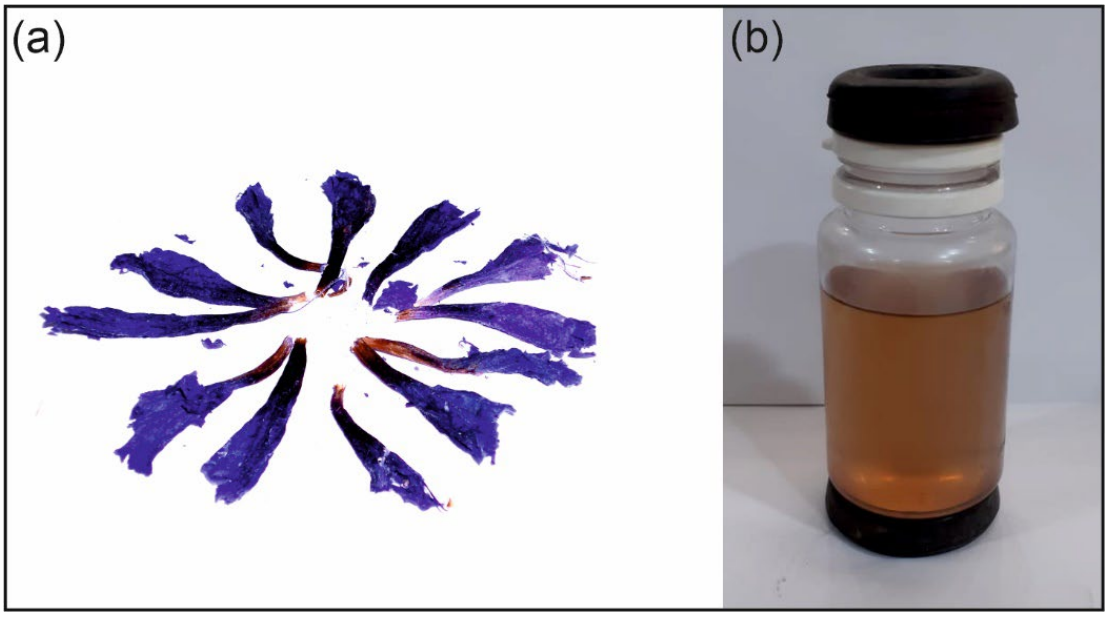

Fig. 1: The materials of extracted dyes used in current study (a) *A.-Italica* flower and (b) configuration of two permanent magnets.

Materials and Methods

Extraction process. The petals of *A. Italica* plant are available at local markets in Iraq. For more details about the checking of the quality and the processes of the dye extraction, the reader can be referred to our work in Ref. [25, 26].

Preparation of the polymer. Pentacene (PEN) ($C_{22}H_{14}$) was provided from Sigma-Aldrich Chemical Co. Ltd. The procedure followed to prepare the PEN sol was also described in Ref. [26].

Aqueous solution magnetization. For a magnetization treatment, a capped plastic container comprising the resulted dye was positioned between two magnets of 5 cm in diameter (KC-70C) which is purchased from the local market in Iraq. At room temperature, the intensity of the magnetic field concentrated at the center position was measured using a digital Gauss/Tesla meter as shown in Figure 1. The magnetization rate of the two toroidal magnets was 1000 ±10% mT and strength of 0.20 T as well. The *A. Italica*-doped PEN solution was subjected to a static magnetic field for no more than 50 minutes.

Preparation of thin-film. A thin film dye/PEN obtained was poured on a 2 × 2 cm glass slide that has been cleaned with distilled water and acetone, dried at 65 ºC, and after that heated for 20 minutes in the oven. The casting step was performed by the spin coating technique for several rotations (1000 rpm/min).

Characterization Techniques

Analysis of stretching mode. The IR-transmission spectrum of both pure PEN and *A. Italica* dye and their information are presented in Ref. [26, 27]. Figure 2 shows the FT-IR spectra of the *A. Italica*-doped PEN, which shows a distinctive band about 3394 cm^{-1} [υ (O–H)], with the spectrum at 2925 cm^{-1} attributable to C-H aliphatic and the implication of C=O group at 1742 cm^{-1}. The bending vibration of the C–O group is responsible for the absorption peak at 1059 cm^{-1}. In addition, the energies at 1440 cm^{-1} and 1350 cm^{-1}, are indicated to the presence of two bending vibrations CH_2 and CH_3 respectively. The main modifications in the Infrared region of the doped sample may be detected in the range of 1000-2000 nm. The transmittance bands of the components are displayed in Table 1.

Table 1: The main IR transmittance bands recorded for the powder compounds.

Compound	υ(O-H) str.	υ (C-H) aliphatic	υ (C=O) str.	υ (C=C) str.	υ (C-O) str.	υ (C-H) aliphatic bend
A. Italica-doped PEN	3394 (br)	2925 (m)	1742 (w)	1627 (s)	1059 (s)	1440 (w)

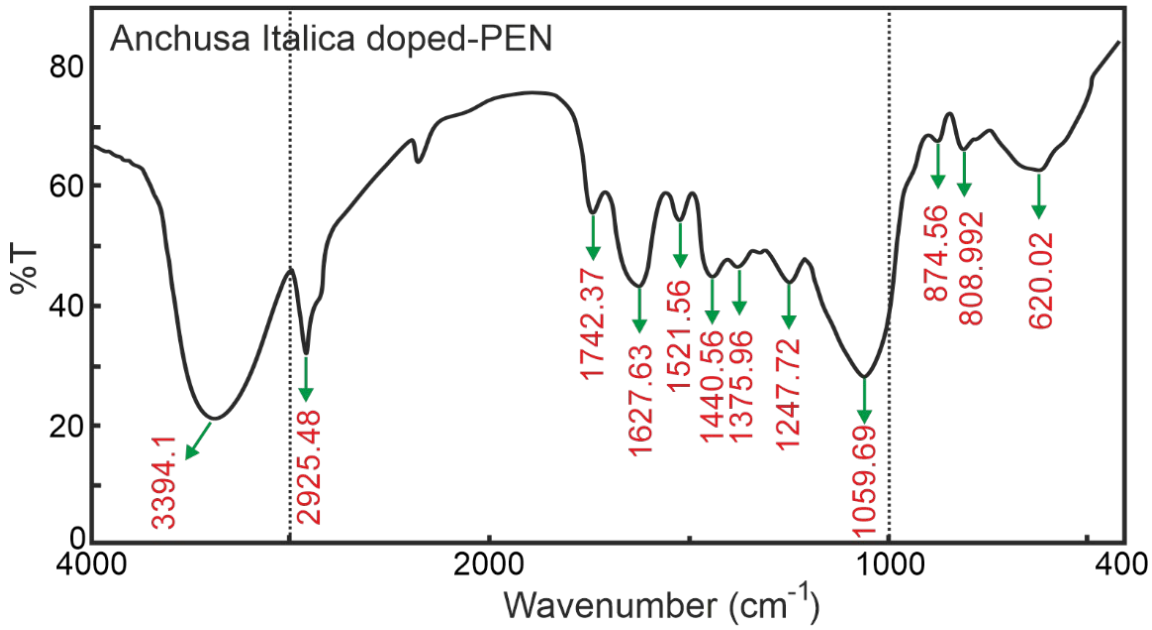

Fig. 2: Fourier transform infrared spectroscopy of dye doped polymer composites.

Results and Discussion

Optical absorbance. Many factors can affect the optical absorption spectrum, including chemical structure, thickness and absorbed light energy of the sample under study. Different UV-visible spectroscopies were carried out at room temperature using a dual light-beam UV-visible spectrophotometer (CE-7200). In our investigation, as we will see later, the presence of a static magnetic field affected the aqueous extract. The absorption spectra of the magnetized *A. Italica*-doped PEN thin film were measured in the range of 300–800 nm. To understand the full implications of the magnetization effect, the absorption spectra of *A. Italica*-doped PEN (ADP) thin film were also recorded as the reference one. Figure 3 shows a comparison of the absorption curves between MADP and ADP samples having the same film thickness. As shown in Figure 3, the absorption maxima of ADP starts at 310 nm and achieves 40% intensity, whereas the spectral postion of MADP is significantly redshifted with 32% intensity.

Optical absorption coefficient. The absorption coefficient becomes particularly significant in the absorption band to identify the kind of electronic transition that occurs in the electronic structure of the substance. To achieve this objective, The following equation was used to estimate the absorption coefficient. [28]:

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

Where T and R represent transmittance and reflection, respectively, while *d* is the thickness of the sample. The factor *d* is obtained from the conventional approach, which involves the use of spectroscopic ellipsometry (SE) equipment (M2000V, J.A. Wollma Co., Inc.). As a result, the thickness of *A. Italica* thin film is 195 mm. The optical energy gap is usually classified using the calculated parameter α.

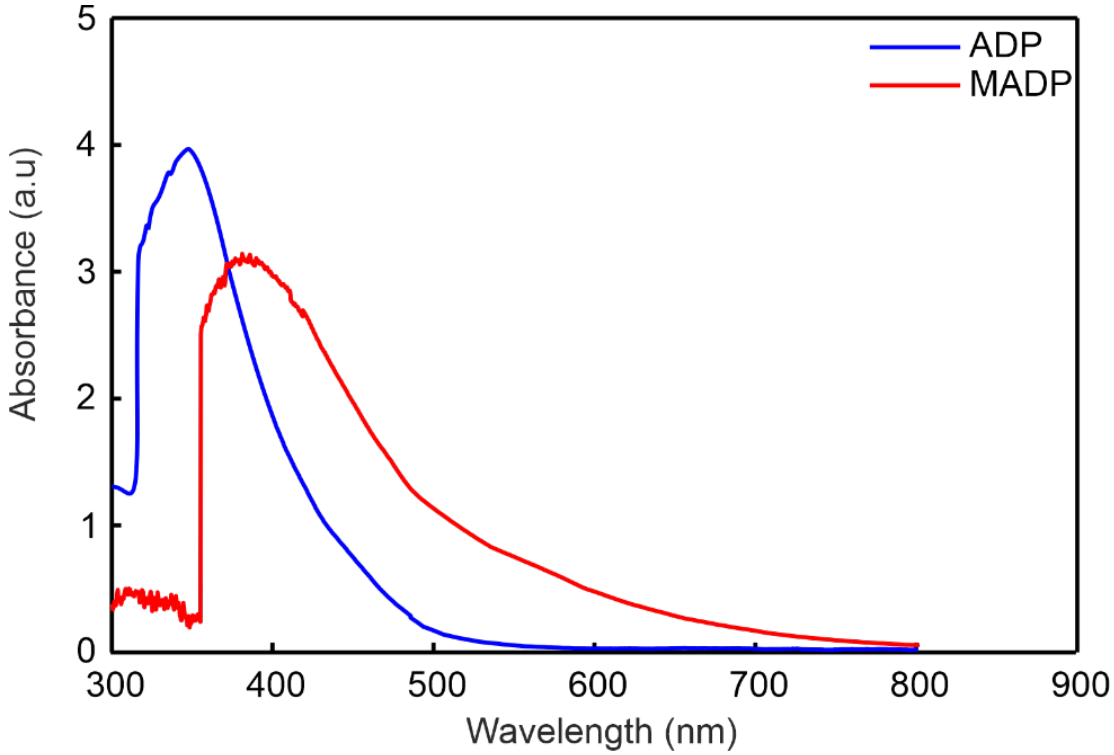

Fig. 3: The absorbance profile of MADP and ADP samples.

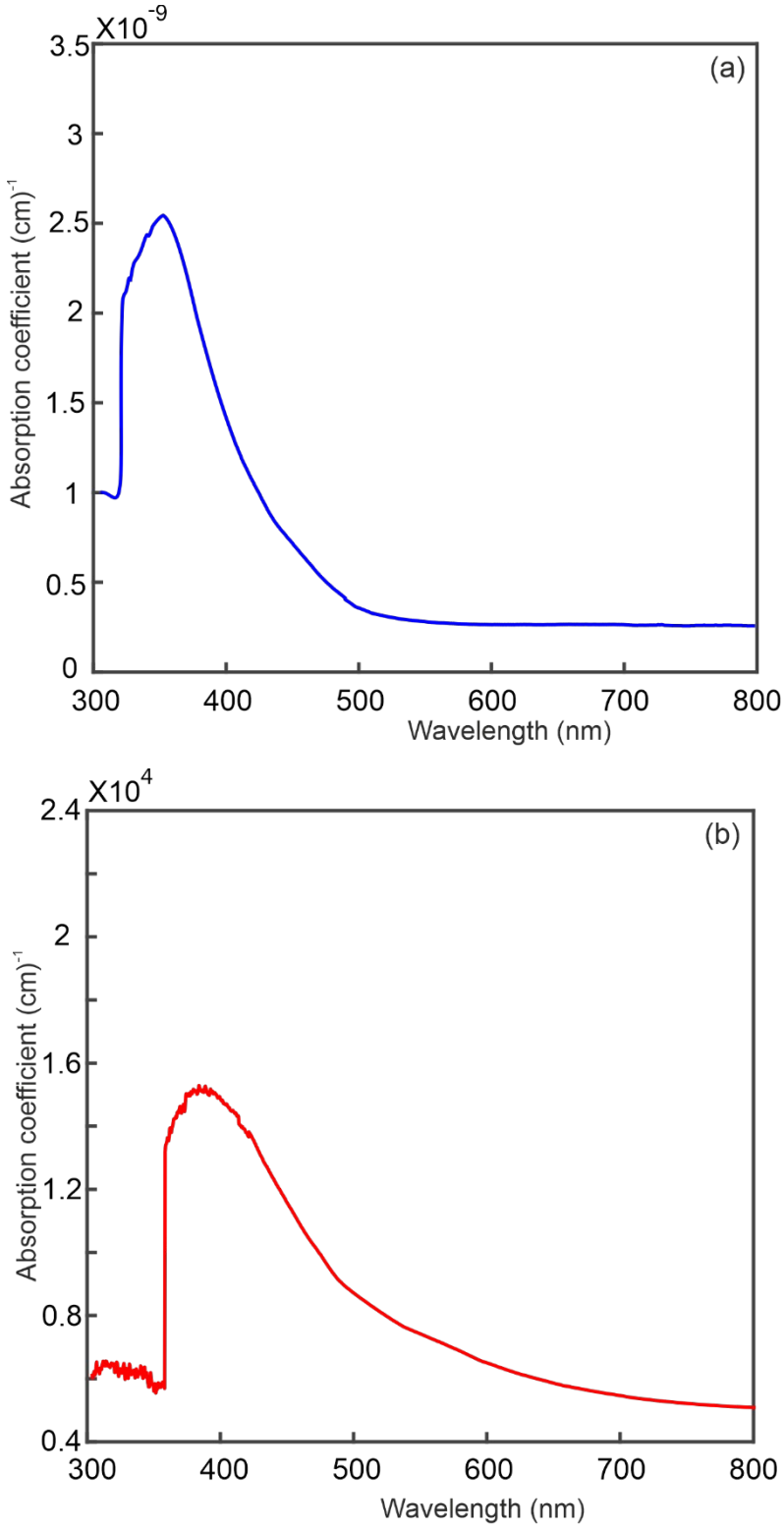

Fig. 4: Absorption coefficient of (a) ADP, and (b) MADP thin-films.

In the 300-800 nm bandwidth, the factor α was evaluated for MADP and ADP with the same film thickness (see Figure 4). One can see, the MADP exhibits a considerable spectral response outperforming the ADP one, due to the electronic properties affected by the static magnetic field. Figure 4(a) illustrates that the peak magnitude of ADP is about ($< 10^4$), demonstrating that electronic transmission between the levels was indirect [28]. In contrast, the peak value obtained of MADP film is different, allowing a direct transmission (see Figure 4(b)). As shown in Figure 3, the energy gap magnitude can be estimated by plotting intercept $(\alpha h\upsilon)^{\gamma}$ vs $h\upsilon$ of the x-axis (i.e. $(\alpha h\upsilon)^{\gamma}=0$). The latter finding, which may be derived from the Tauc's relationship as follows [29, 30]:

$$\alpha = \frac{A[(h\upsilon - E_g)]^{\gamma}}{h\upsilon} \quad (2)$$

where A is the transition probability dependent factor, and γ represents the density of states index distribution, which might have different values corresponding to the transition path (γ= 2 or 3 and γ= 1/2 or 3/2 for direct and indirect transition paths respectively)

Optical energy gap. In terms of the energy gap, calculating the photon output in the visible range is also interesting. Such photons are in charge of causing the electron to be excited to atomic energy states in the conduction band. Consequently, as the energy bandgap narrows, the number of unoccupied states in that band increases. To demonstrate how to calculate the bandgap energies of thin films, Eq. 2 mentioned above is used and the value of the γ index is included as well. As shown in Figure 5(a), the electronic transition was indirect which allows Tauc's relationship to be proportional with $(\alpha h\upsilon)^2$. The ADP sample exhibits an energy gap (E_g) with a magnitude of 2.61 eV, as illustrated in Figure 5(a). The result confirms the presence of defects in the sample which allow to appear some distinct sub-levels just under the conventional conduction band. One can demonstrate from Fig. 5(b) that the magnetization effect leads to a smaller energy gap value (E_g=1.76 eV) of the MADP sample. The modification in the latter value is linked to the OH content which indicates that the magnetic field yields more molecular dipoles and coherent energy approaches.

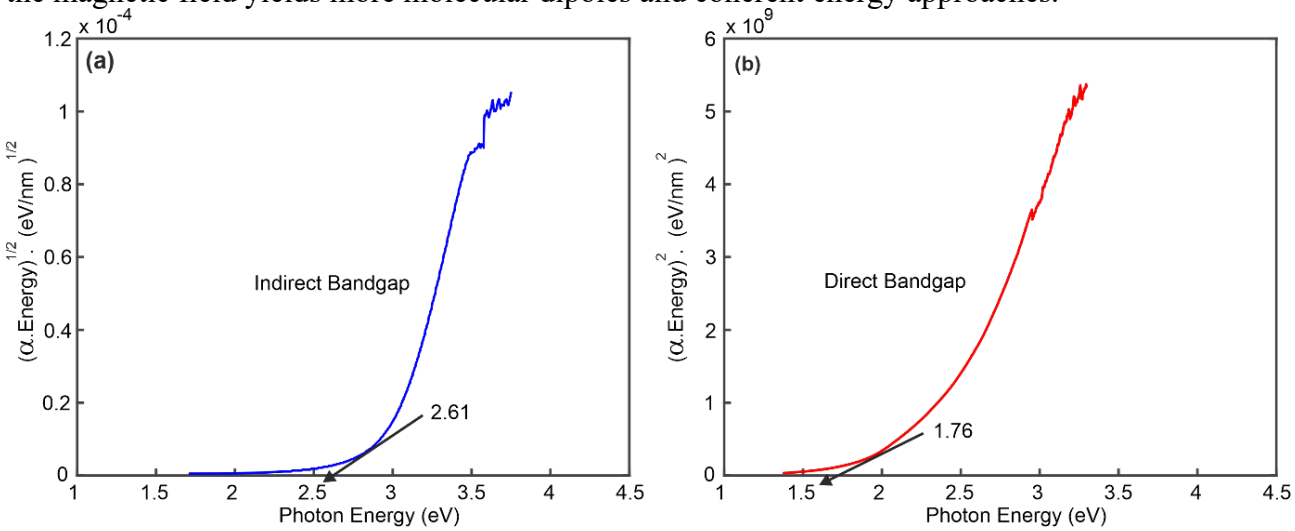

Fig. 5: Energy bandgap of (a) ADP, and (b) MADP thin-films using Tauc relation.

Linear refractive index (n) and extinction coefficient (k). There are other important coefficients (*n* and *k*) that play a vital role and govern the optical properties of optoelectronic systems. This role is attributed to the interbond of electrons transition from valance to conduction band. The following relationships can be used to determine the two quantities *n* and *k*.

$$k = \frac{\alpha\lambda}{4\pi} \quad (3)$$

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

Figure 6(a) depicts the relationship of index *n* versus the wavelength for the ADP and MADP samples to determine how the magnetization affects the index *n*.

The results show that the refractive index of the ADP thin film gradually increased in the range of 350 ~ 450 nm as shown in Fig. 6(a) (the blue curve). As the spectrum moves towards the low energy region, the factor *n* exhibits a dropping behavior. Figure 6(a) depicts a development in the refractive index spectrum within the MADP film of 580 nm in wavelength, which continues the linear increase throughout the bandwidth. On the other hand, the optical response of the absorption spectrum shows the action of the real part of the index *n* in Fig. 6(a) (red curve),

confirming the resonance mode in the MADP thin film. The second important factor is the extinction coefficient *k* which plays a key role in the spectrum region as presented in Eq. 3. As shown in Fig. 6(b), the index *k* for both ADP and MADP samples are measured in the mid to high-frequency region. The absorption index of MADP film has a lower spectral response than the ADP thin film (see the red curve in Fig. 6(b)). As a result, light penetrates the MADP thin film with minimal attenuation, which is specifically linked to the material's dispersion properties, which are controlled by the polarization effect and dielectric losses.

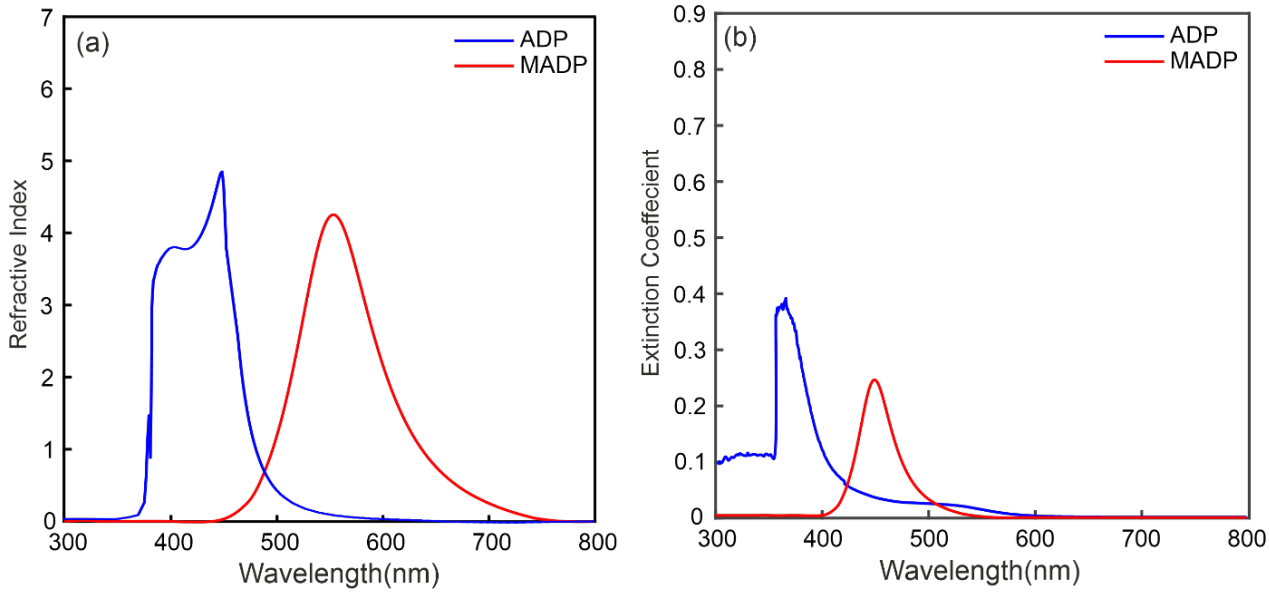

Fig. 6: (a) Refractive index and (b) the extinction coefficient of ADP and MADP samples.

Conclusion

In conclusion, the absorbance, absorption coefficient α, band gap edge, refractive index *n*, and extinction coefficient *k* were investigated with and without the magnetization effect. The absorption maxima of the MADP sample displays a red-shifted part as compared with the normal (ADP) high-frequency region. The obtained results explain that the magnetic field applied plays a vital role in the magnetic dipole-momentum of electrons and the polarization in molecules of the material's sample. In the MADP sample, the direct transmission was found due to the α magnitude ($< 10^4$), whereas indirect transmission was confirmed in the ADP sample. The optical bandgap was reduced from 2.61 to 1.76 eV via magnetization and converted to a direct band gap. The obtained study of the refractive index performed on the samples exhibits an increasing near-blue region for the MADP sample and a quasi-stability in the low energy region for the ADP sample. In terms of extinction index, a quite low-light attenuation was generated in the MADP sample due to the change in dispersion characteristics caused by the magnetization.

Acknowledgments

The Polymer Research Center at the University of Basrah has contributed to this work by performing the required measurements and providing experimental materials.

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