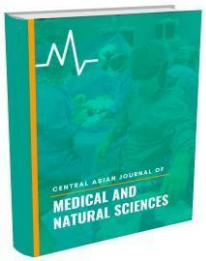

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Article

An Experimental Study of Some Optical Properties of The Organic Semiconductor Molecule (Alq3)

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Abstract: In this research, an experimental study was conducted to analyze the spectral effects of different concentrations of the organic semiconductor Tris(8-hydroxyquinoline)aluminum (Alq_3), using UV-Vis absorbance measurements in the spectral range of (200–1100) nm. Three samples were prepared with concentrations of (0.01, 0.02, 0.03) mM and a set of main optical properties were analyzed, including the absorption coefficient (α), refractive index (n), optical extinction coefficient (k), real (ε_1) and imaginary (ε_2) dielectric constants, in addition to optical conductivity (σ_o).The results showed that increasing the concentration of Alq_3 leads to a significant improvement in photon absorption and intensification of the optical response, attributed to enhanced molecular packing and increased density of optically active centers. Additionally, distinct electronic transition peaks of the $\pi^*\rightarrow\pi$ and $n^*\rightarrow\pi$ kinds were detected, indicating the possibility of improving the material's optical qualities for use in organic optical devices including organic solar cells and light-emitting diodes (OLEDs). This study emphasizes how crucial it is to regulate the material's concentration as a useful factor for precisely adjusting its electrical and spectral characteristics.

Keywords: Absorption Coefficient, Dielectric Constant, Optical Extinction Coefficient, Optical Conductivity, Organic Semiconductor, Refractive Index

1. Introduction

Alq3, or tris (8-hydroxyquinoline) aluminum (III)

An organometallic molecule known as tris (8-hydroxyquinoline) aluminum (III), or Alq3, is mostly utilized in organic electronics applications, particularly in the production of organic light-emitting devices (OLEDs). Because it has an aluminum atom encircled by three 8-hydroxyquinoline molecules—organic molecules having a quinoline ring with a hydroxyl group (OH-) at position 8—this compound has a distinctive chemical structure. This compound's unique chemical, see Figure 1 and physical characteristics, which come from its molecular structure, make it a perfect fit for a wide range of cutting-edge technological applications [1].

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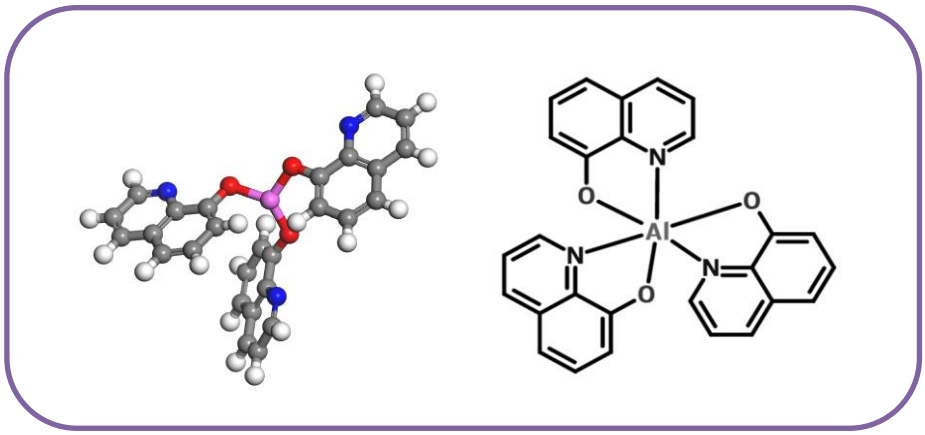

Figure 1. is the chemical structure of Alq3 [2].

Because of its highly valued optical and electrical qualities, including brightness, electrical conductivity, and affordability, Alq3 has become more and more popular among scientists [3]. As a result, this material is crucial for electronic and optical applications such photovoltaic cells, flat and flexible color displays, and OLED panels, see Table 1. In 1987, it was shown that Alq3 might be used to create a high-brightness, low-voltage device [4]. Since then, every effort has been made to advance the technology of organic light-emitting diodes, or OLEDs [5]. Alq3 is regarded as one of the most effective materials for organic light-emitting diode (OLED) applications and is among the most stable materials that may be utilized to build thin films on plastic substrates. Enhancing the device's characteristics has been the focus of recent research [6].

Table 1. Physical properties of Alq3 [7].

$C_{27}H_{18}AlN_3O_3$	**Molecular formula**
Greenish-yellow powder	Appearance
1.35 g/cm^3	Density
415.4 °C	Melting point
459.43 g/mol	Molar masses

2. Materials and Methods

According The practical part

UV absorbance measurements

Before measuring the UV absorbance, three samples of the study material are prepared. The molecule we are studying is tris(8-hydroxyquinolinato)aluminum (Alq3), as shown in Figure 2. Where the preparation is done by dissolving (Alq3) in distilled water at concentrations of (0.1 mM), (0.2 mM), and (0.3 mM). Through this dissolution, three samples are obtained, which are then examined using the UV absorbance measurement device.

Figure 2. Study Material (Alq3).

The prepared samples were taken and measured (UV-visible) in the laboratory, where the examination was conducted at room temperature using the Lambda 365 Perkin Elmer device shown in figure 3 within the absorption range (190 – 1100 nm) with a double beam. In this measurement, the absorption spectra as a function of photon energy for the three samples that were examined were shown.

Figure 3. UV spectrophotometer.

Optical properties

The absorption coefficient can be defined as the ratio of the decrease in the flux of incident radiation energy to the distance in the direction of wave propagation within the medium. The absorption coefficient depends on the properties of the material and the energy of the photon in terms of the energy gap and the type of electronic transitions. The absorption coefficient (hv) is given by the following relationship [8].

$$E = hv \qquad (1)$$

If the forbidden energy gap is greater than the energy of the photon, there will be an electron transition, where the permeability is given by the following equation[9]:

$$T = (1 - R)^2 \, exp(-\alpha \, d) \qquad (2)$$

Where / **d** represents the sample thickness, $\boldsymbol{\alpha}$ the absorption coefficient, **T** the transmittance, and **R** the reflectance.

The intensity of the light transmitted through the thickness of the slide when light falls on the slide is given by the following relationship [10].

$$IT = I_o\, exp(-\alpha d) \quad (3)$$

$$IT / I_o = exp(-\alpha d) \quad (4)$$

Since : $T = IT / I_o$

$$T = exp(-\alpha d) \quad (5)$$

$$1/T = exp(\alpha d) \quad (6)$$

$$\alpha d = 2.303 log\ (I_o / IT) \quad (7)$$

Since : $A = log(I_o / IT)$

$$\alpha d = 2.303 \times A \quad (8)$$

$$\alpha = (2.303 \times A)\ / d \quad (9)$$

Where A represents the absorption of the material for the incident light, and d represents the thickness of the sample in (cm) units.

One of the most important properties of an optical medium is the refractive index, which can be defined as the ratio of the speed of light in a vacuum to the speed of light in the medium. It is given by the following equation [11].

$$n = \frac{c}{v} \quad (10)$$

Since the refractive index (n) is approximately greater than one and depends on the temperature [12], and the refractive index of the polymer also varies directly with the medium's density.

The electromagnetic wave in the material suffers from attenuation, meaning a loss of energy, which is called the attenuation coefficient. It can also be expressed as the amount of loss in the energy of the electromagnetic wave when it enters the material [13].

In the complex refractive index, the imaginary part is called the extinction coefficient as shown in the following relation [14].

$$n = \frac{c}{v} = n - ik_o \quad (11)$$

Where ((n represents the real part of the refractive index. The attenuation coefficient can be calculated using the following relationship [15].

$$k_o = \frac{\alpha\lambda}{4\pi} \quad (12)$$

Where (λ) represents the wavelength of the incident ray on the material. The dielectric constant (ε) can be defined as the measure of the material's insulation, and the dielectric constant can be calculated through the refractive index. Where the real permittivity and the imaginary permittivity can be calculated using the following equations [16]:

$$\varepsilon = \varepsilon_1 - i\varepsilon_2 \quad (13)$$

$$(n - ik)^2 = \varepsilon_1 - i\varepsilon_2 \quad (14)$$

$$n2 - 2nki - k2 = \varepsilon_1 - i\varepsilon_2 \quad (15)$$

Where the real insulation coefficient and the imaginary insulation coefficient can be written as follows:

$n^2 - k^2$) (16)$_1\varepsilon$=(

nk) (17)$_2\varepsilon$= (2

Where: 1ε represents the real dielectric constant, 2ε represents the imaginary dielectric constant.

Through the following relationship, the optical conductivity can be found, where it is measured in the unit (1/s) [17].

$$\sigma_{op} = \frac{\alpha\, n\, c}{4\pi} \quad (18)$$

3. Results and Discussion

Figure 4 shows that the change in the absorption coefficient (α) in units of cm^{-1} for an Alq_3 sample dissolved in distilled water at three different concentrations (0.01, 0.02, 0.03 mM) as a function of photon energy (E) within the range (1 – 7 eV). It is observed from the

curves that a distinctive behavior is associated with the change in electronic structure due to the variation in concentrations.

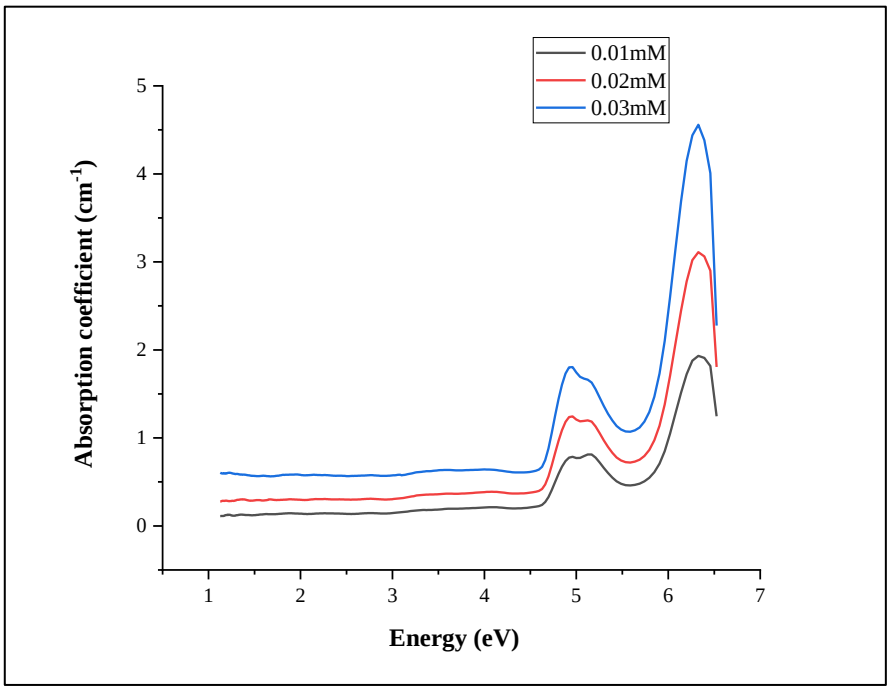

Figure 4. Absorption coefficient as a function of photon energy for the organic semiconductor molecule (Alq3).

The curves show a gradual increase in the absorption coefficient values with the increase in light energy, and it is clear that the value of (α) increases as the concentration of the material increases, and it also increases with the increase in photon energy, as noted in previous studies [18].This indicates that increased concentration enhances the material's ability to absorb photons in specific energy ranges, reflecting an increase in the density of electronic states or the number of optically active centers within the material.

The curve can be divided into three main regions:

• **The first region:** (E < 4.5 eV): The absorption is very weak, representing what is known as the optical transparency region of the material.

• **The second region:** approximately at (E= 5.2 eV) the first clear jump in absorption begins, indicating the start of $\pi \rightarrow \pi^*$ electronic transitions associated with the aromatic structure of Alq_3.

• **The third region:** approximately at (E=6.3 eV) represents the peak absorption, and it is believed to be associated with electronic transitions from non-bonding orbitals (n) or to higher energy conduction levels, as reported in similar studies on Alq_3 and its derivatives [20], [19].

The height of the absorption peaks increases significantly when moving from 0.01 mM to 0.03 mM, indicating that the increase in concentration improves the interaction between molecules and enhances electronic conductivity and π-orbital overlap, which is reflected in the improved absorption properties.Previous studies have shown that increasing the concentration in polymers and organic semiconductors contributes to improving optical activity and increasing absorptivity[21]. These results indicate the possibility of using higher concentrations of the additive to improve the optical performance of Alq_3 in organic electronics applications, such as light-emitting diodes (OLEDs), photodetectors, and organic solar cells.

Figure 5 quantitatively illustrates the change in the refractive index (n) of the compound Alq_3 using UV-Vis technique within the spectral range (200–1100 nm), at three different concentrations of the additive (0.01, 0.02, 0.03 mM).

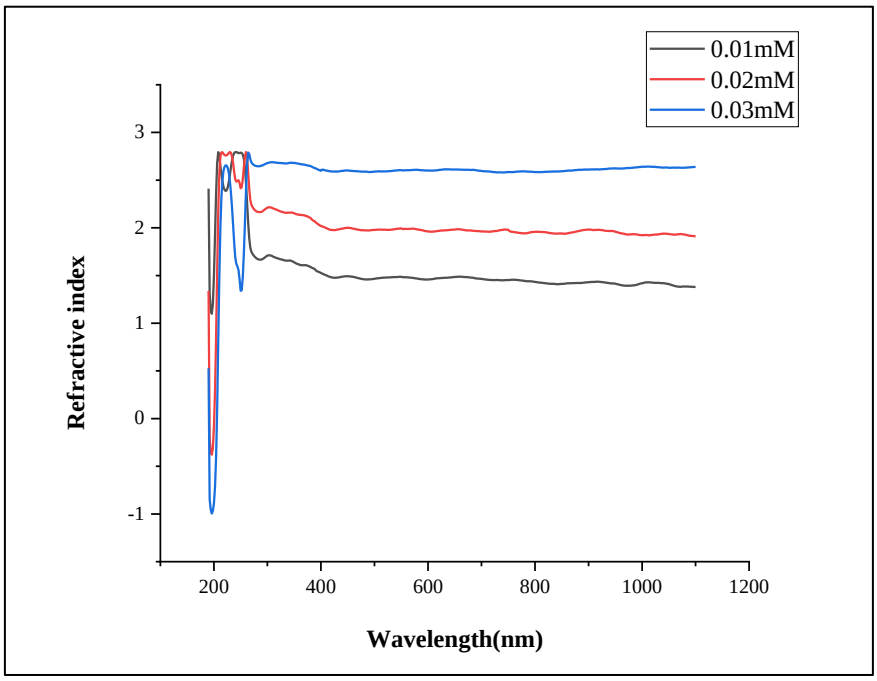

Figure 5. The refractive index as a function of wavelength for the organic semiconductor molecule (Alq3).

It was observed that all samples exhibit a common behavior characterized by a sharp decrease in the refractive index within the ultraviolet region (200–300 nm), followed by relative stability in the visible and near-infrared spectrum.This behavior is attributed to the sharp decrease in the absorption coefficient due to the displacement of the optical energy from the absorption edge, which is consistent with the nature of organic semiconducting materials.

It is also observed that there is a direct relationship between the concentration of the added substance and the refractive index; the value of n increased with the concentration.For example, at a wavelength of 600 nm, the refractive index values were approximately 1.6, 2.1, and 2.8 for the concentrations of 0.01, 0.02, and 0.03 mM, respectively.This increase is attributed to the higher optical polarizability of the molecules resulting from the increased density in the structure, which contributes to the improved electronic transition within the molecular network.

During the analysis of the spectral data extracted from UV-Vis measurements, negative values were observed in some reflectivity values.This behavior is attributed to physical and technical effects related to the measurement system, and it can be explained as follows:

When the absorption ratio is very close to zero, the signal measured at the detector becomes extremely low, making it more susceptible to background noise or unwanted electronic currents such as dark currents or vibrations from the power source. In such cases, the ratio between the intensity of the incident and transmitted radiation can be misleading or shift away from zero due to noise effects, resulting in negative values.

Figure (1-6) shows the extinction coefficient (k) curves as a function of wavelength for the Alq_3 sample after dissolving the material at different concentrations (0.01, 0.02, 0.03 mM). The curve shows a distinctive optical behavior that reflects the material's response to light within the ultraviolet and visible spectrum, and demonstrates the extent of concentration's impact on the optical properties of the samples.

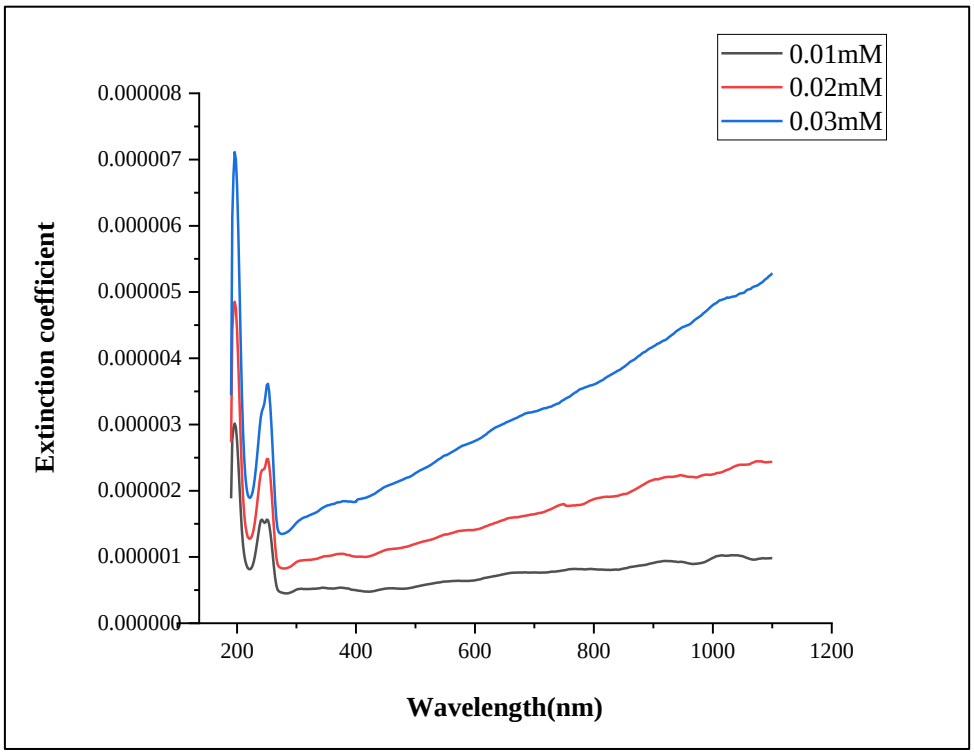

Figure 6. The damping factor as a function of the wavelength for the organic semiconductor molecule (Alq3).

Sharp and clear peaks appear in the region between 200–300 nm for all concentrations, which are associated with $\pi \rightarrow \pi^*$ electronic transitions.Within the aromatic molecules of the Alq_3 compound, these transitions are a direct indicator of the presence of an extended electronic system within the material's structure, which aligns with what has been reported in the previous literature regarding the properties [22].

Alq_3, It is observed that the increase in concentration from (0.01 to 0.03) mM led to a significant increase in the value of the extinction coefficient, especially in the region below 400 nm.This indicates an increase in the optical absorbance of the material with higher concentration, which may be attributed to the following:

- **Increased density of opto-active centers** due to the introduction of higher concentrations of the material.
- **Enhancing molecular packing** within the Alq_3 structure, which improves π-orbital overlap and consequently increases the likelihood of electronic transition[23].

All the curves show a gradual decrease in the damping factor with increasing wavelength, reflecting a decrease in absorptivity at longer wavelengths. This behavior aligns with the traditional characteristics of organic semiconductors with a wide energy gap, where strong absorption is concentrated at shorter wavelengths.

From all of the above, we conclude that any increase in absorption (α) due to changes in composition or concentration will directly reflect an increase in the damping coefficient.

Figure 7 shows that the real part of the dielectric constant (ε_1) clearly changes with the concentration of the Alq_3 material.The sample with a concentration of 0.01 mM (black color) shows the lowest values of ε_1 at low energies, while this value gradually increases with the concentration to 0.02 mM (red color) and 0.03 mM (blue color), reaching the highest value in the range between (5.5 –6.5)eV.

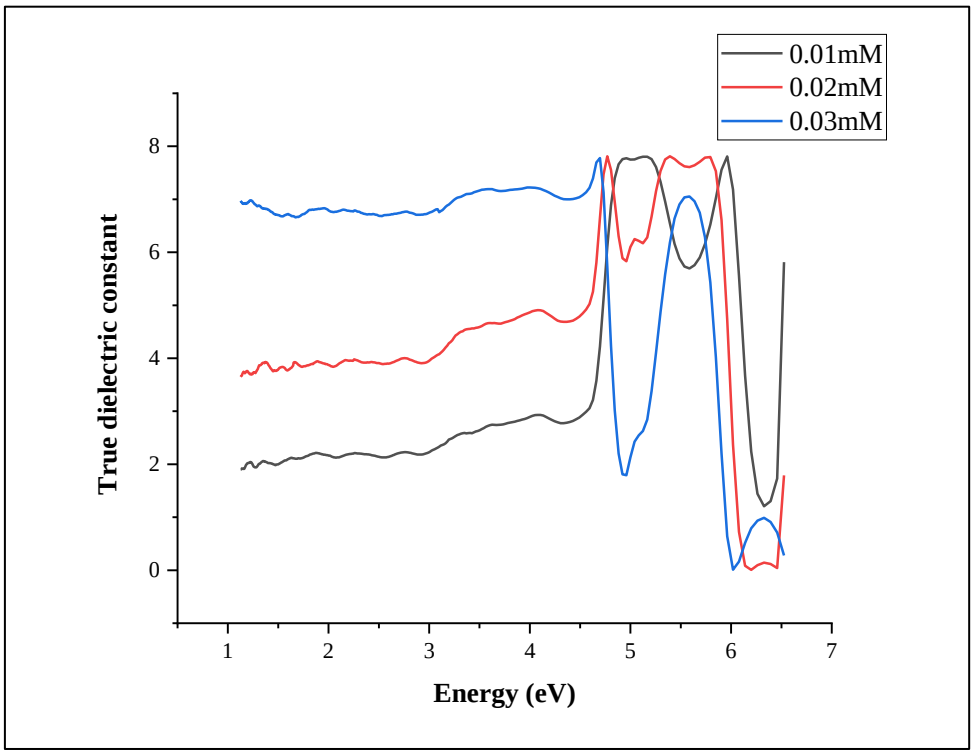

Figure 7. The real dielectric constant as a function of energy for the organic semiconductor (Alq3).

The real part of the dielectric constant indicates the polarization of the material in the electric field without actual light absorption. Therefore, the increase in ε_1 values at higher concentrations means an increased ability of the material to respond to the photonic electric field, which may be related to an improvement in the arrangement of molecules or the density of electronic bands at the highest concentrations.

Distinct peaks were observed at approximately 5.3 eV and 6.1 eV, which represent regions of strong interaction between photons and the electronic structure of the material. These peaks rise and become more noticeable as concentration increases, suggesting that dissolution at greater concentrations has improved optical characteristics.

These findings align with previous research, since one study [25] found that enhanced polarization within the material in response to higher concentrations causes an increase in ε_1.

Based on this, we deduce that an improvement in conductivity and polarization characteristics is indicated by a rise in ε_1 at greater concentrations. Furthermore, the development of sharper peaks at a concentration of 0.03 mM would indicate that the bonds between Alq_3 molecules are getting stronger.

For Alq_3 membranes dissolved in three distinct concentrations (0.01, 0.02, and 0.03) mM, the change in the imaginary portion of the dielectric constant (ε_2) as a function of photon energy is shown in Figure (1–8). These values were obtained through UV-Vis measurements, without any distortion of the sample, but rather due to the change in the concentration of the organic semiconductor only.

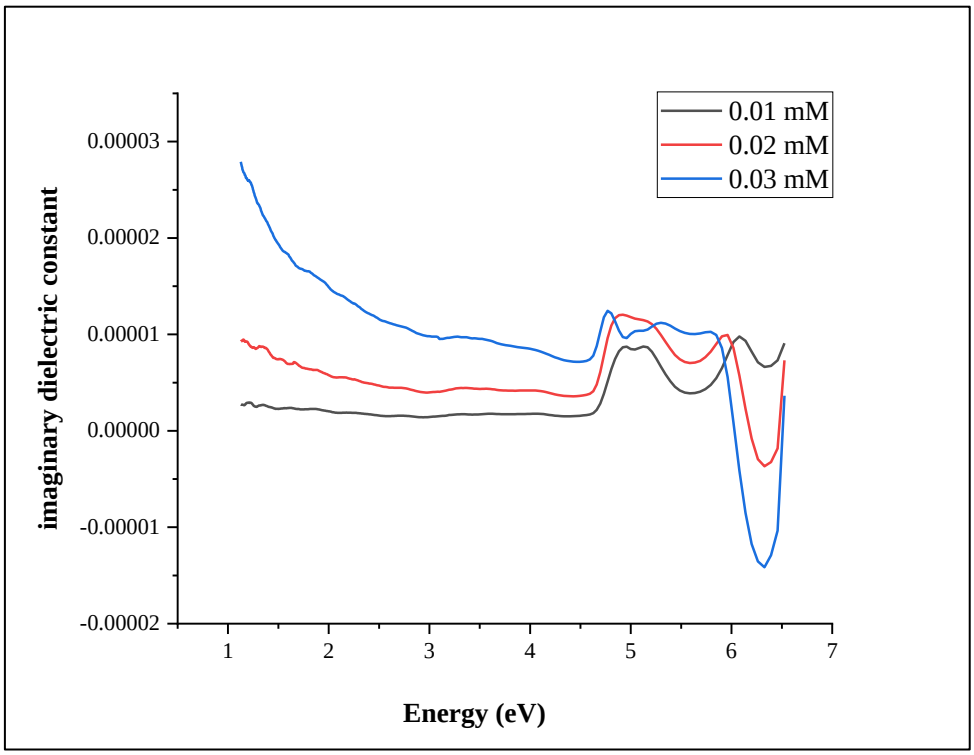

Figure 8. The imaginary dielectric constant as a function of energy for the organic semiconductor (Alq3).

It is observed that the value of ε_2 begins to gradually decrease with increasing photon energy in the range from 1 eV to 4 eV, which is a typical behavior resulting from reduced absorptivity at these low energies.Then, clear peaks appear in the range between 5 eV to 6.5 eV, indicating strong electronic transitions between the molecular orbitals $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$.

It is worth noting that the value of ε_2 increases with the concentration of the substance, with the sample at a concentration of 0.03mM showing the highest values of the imaginary constant across most of the spectral range, followed by 0.02 mM and then 0.01 mM. This phenomenon is explained by the higher likelihood of electronic transitions brought about by better molecule packing and stronger orbital overlap, as well as the larger density of electronic states accessible for absorption.

Some reflectivity readings showed negative values when the spectral data from UV-Vis measurements was analyzed. The following explanation explains this phenomenon, which is caused by technical and physical phenomena associated with the measuring system:

The detector's signal is very low when the absorption ratio is very near zero, which leaves it vulnerable to undesired electronic currents like dark currents or power source vibrations as well as background noise. In certain situations, the ratio of incident to transmitted radiation intensity may be deceptive or deviate from zero because of noise effects, producing negative readings.

These results are consistent with what was reported in one of the studies [26], which indicates that the imaginary part of the dielectric constant is directly related to the material's absorption and is considered an important indicator of electronic transition activity within the molecular structure.

Therefore, the results confirm the possibility of controlling the optical dielectric properties of Alq_3 films by adjusting the material concentration, which allows for improved performance in optical and electronic applications, particularly in OLED devices and solar cells.

Figure 9 shows the optical conductivity curves of Alq3 films with different material concentrations, with these concentrations (0.01mM, 0.02mM, 0.03mM) represented in black, red, and blue, respectively, as a function of photon energy.

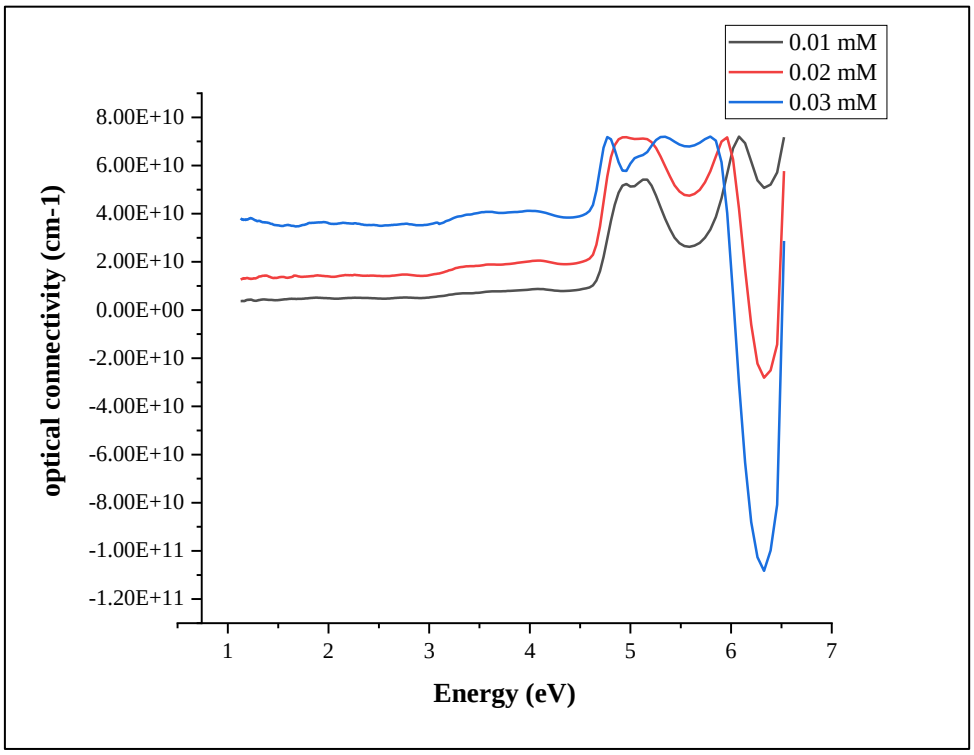

Figure 9. Optical conductivity as a function of energy for the organic semiconductor (Alq3).

The results show that the optical conductivity is relatively low at low energies and begins to gradually increase with the increase in photon energy, recording a noticeable jump at approximately 5 eV and reaching maximum values in the range of (6.0 – 6.3 eV), indicating strong electronic transitions at these energies.

It was observed that increasing the concentration of the material from 0.01 mM to 0.03mM leads to a significant increase in optical conductivity across the entire spectral range, with the sample at 0.03mM showing the highest conductivity, followed by 0.02mM and then 0.01mM.This behavior is attributed to the increase in the density of electronic states available for excitation, as the improvement in conductivity is related to the enhancement of molecular order within the structure, leading to increased overlap between π orbitals and higher efficiency of $\pi \rightarrow \pi^*$ transitions.

During the analysis of the spectral data extracted from UV-Vis measurements, negative values were observed in some reflectivity values.This behavior is attributed to physical and technical effects related to the measurement system, and it can be explained as follows:

When the absorption ratio is very close to zero, the signal measured at the detector becomes extremely low, making it more susceptible to background noise or unwanted electronic currents such as dark currents or vibrations from the power source. In such cases, the ratio between the intensity of the incident and transmitted radiation can be misleading or shifted away from zero due to noise effects, resulting in negative values.

These findings are in line with earlier research, which found that boosting optical transitions at specific wavelengths and altering the electrical structure by doping at low concentrations can enhance optical conductivity in organic semiconductor systems [22]. Increased doping in the compound Alq3 also improves optical and electrical characteristics by increasing the amount of free carriers and improving molecular interactions, according

to another research [27]. By increasing the amount of free carriers and improving molecular interactions, doping the Alq3 compound improves its optical and electrical characteristics.

Therefore, the current results confirm that modifying the concentration of the additive is an effective means of adjusting the optical properties of Alq3 films, which serves their applications in optoelectronic devices such as organic light-emitting diodes (OLEDs).

4. Conclusion

Based on the spectral results obtained from the analysis of Alq_3 samples at different concentrations, the following conclusions can be drawn. FirstImprovement of absorptivityThe absorption coefficient (α) curves showed significant increases with higher concentration, especially in the energy range (5–7) eV, indicating an increased probability of photon absorption and electron transitions through molecular orbitals, which is a sign of enhanced electronic density within the structure.Secondly, the enhancement of electronic transitions, as the appearance of sharp absorption peaks at specific energies (5.2 and 6.3 eV) reflects effective electronic transitions of the $\pi^* \rightarrow \pi$ and $n^* \rightarrow \pi$ types, becoming more pronounced with increasing concentration, indicating an improvement in the organization of molecular orbitals.And thirdly, in the refractive index and extinction coefficient, the measurements showed an increase in the refractive index (n) and extinction coefficient (k) with higher concentrations, especially at shorter wavelengths, which is attributed to the increased polarization of the medium and improved overlap of electronic orbitals.Similarly, analysis of the real (ε_1) and imaginary (ε_2) dielectric constants showed that the values increase significantly with higher concentrations, reflecting a greater ability of the material to respond to the photonic electric field without significant energy loss, which confirms an improvement in charge dynamics.We also conclude that the increase in optical conductivity (σ_o) at high energies is proportional to the concentration of the material, which is attributed to the enhanced molecular ordering and the increased density of excitably electronic states.The results also confirm that controlling the concentration of Alq_3 provides an effective means to adjust its spectral properties, enhancing its potential for use in optoelectronic applications, particularly OLEDs, photodetectors, and organic solar cells.Accordingly, the study recommends using carefully controlled concentrations of Alq_3 as a key factor to enhance optical performance in organic semiconductor systems.

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