Study on Optical Constants and Refractive 
Index Dispersion of Neutral red Doped Polymer Film

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Abstract: Problem statement: The some optical constants polymer thin film with red dye 3-amino-7-dimethylamino-2-methyl phenazine (NR) as the guest material and Polyvinylpyrrolidone (PVP) as the host material were prepared by adulteration and spin-coating methods. Approach: The values of some important parameters (refractive index \( n \), extinction coefficient \( K \) and dielectric constant \( \varepsilon_{\infty} \)) of polymer thin film are determined from these spectra. Results: It has been found that the dispersion data obey the single oscillator relation of the Wemple-DiDomenico model, from which the dispersion parameters and high-frequency dielectric constant were determined. The estimation of the \( E_0 \), \( E_d \) and \( \varepsilon_{\infty} \) are 1.27, 3.175 and 3.5 eV respectively. Conclusion: The single oscillator model was used to calculate their optical constants from the transmittance and reflectance spectra. The dispersion of the refractive index in film follow the single electronic oscillator mode relation. The UV-Visible spectroscopic studies showed that, the NR film have high refractive index and high dielectric constant. The variation of the dielectric constant with the wavelength indicates that some interactions between photon and electrons in the films are produced in this wavelength range. These interactions are observed on the shapes of the real and imaginary parts of the dielectric constant and they cause the formation of peaks in the dielectric spectra which depends on the material type.

Key words: Optical properties, Thin film, azo dye, Polyvinylpyrrolidone (PVP), Neutral Red (NR), phenazine doped, extinction coefficient, dielectric constant, polymer thin film, dispersion parameters

INTRODUCTION

The process of thin film deposition involves the deposition of material atom-by-atom, molecule-by-molecule, ion-by-ion or cluster of species by cluster of species condensation (Preoneanu et al., 1995; Koksbang et al., 1994). This methodology is applied extensively in the manufacture of photocells and is being used in optical coating, microelectronics, surface science engineering and other technologies (Krunks and Mellikov, 1995; Susilawati and Doyan, 2009; Supa’at et al., 2008).

The investigation of the optical constants such as refractive index, extinction coefficient and dielectric constant of the 3- amino-7-dimethylamino-2-methyl phenazine doped polymer film are important for designing of new materials. Optical constants include the valuable information for technological applications. Furthermore, the changes in refractive index are important for controlling optical properties of thin polymer. Optical properties of any organic thin films are important for optical applications, because optical properties are directly related to their structural and electronic properties. The main aim of this study is to investigate the optical properties of polymer thin film with 3- amino-7-dimethylamino-2-methyl phenazine using the optical spectra.

MATERIALS AND METHODS

The molecular structure of 3- amino-7-dimethylamino-2-methyl phenazine (Neutral Red) is shown in Fig. 1. In our experiment, the host material is Polyvinylpyrrolidone (PVP) and the ratio of Neutral Red in PVP by weight is 0.6%. The NR-doped PVP films were prepared as follows: Neutral Red and PVP are dissolved separately in distilled water and then the solution of Neutral Red (NR) and that of PVP are mixed, heated (up to 50°C) and stirred for 2 h; thus the mixed sols of NR and PVP were obtained. After the sols were filtrated, the films were prepared on a clean glass slide by the repeat-spin-coating method and dried at room temperature for 48 h. The thickness of the film is about 0.7 \( \mu \)m and the film samples have good purity and uniform thicknesses.

The absorption spectrum of the film sample is shown in Fig. 2, where the peak of absorption is located at 533 nm. In addition, our experimental results show that 3- amino-7-dimethylamino-2-methyl phenazine doped. Polymers have a stronger photo-induced birefringence effect (El-Nahass et al., 2010).
RESULTS AND DISCUSSION

Dielectric constant:

**Refractive index dispersion**: Figure 3a and b show the transmittance and reflectance spectra of the 3-amino-7-dimethylamino-2-methyl phenazine. As seen in figures, the direct electronic transitions from \( \pi \) to \( \pi^* \) orbital’s in the 300-450 nm range results in an intense band called the Soret band, which gives the absorption edge in 3-amino-7-dimethylamino-2-methyl phenazine (Unni and Menon, 2000). The other band of the NR is the Q-band, which appears in the region between 550 and 750 nm.

The reflectance spectrum was used to calculate the refractive index of the NR. The refractive index can be determined from the following Eq. 1 relation (Farag and Yahia, 2010):

\[
R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}
\]  

(1)

where, \( k \) is the extinction coefficient and was calculated using \( k = \alpha \lambda /4\pi \). Figure 4a and b show the real and imaginary parts of the refractive index of the NR. It is seen that the refractive index \( n \) changes with the wavelength and shows peak. In the region between 550 and 750 nm a Q band was observed.
Fig. 5: plot of \(1/(n^2-1)\) Vs \((\nu h)^2\)

Table 1: The optical parameters of the film

| Sample | \(E_0\)(eV) | \(E_d\)(eV) | \(n(0)\) | \(S_0\)(m\(^2\)) | \(M_{-1}\) | \(M_{-3}\)(eV)\(^2\) |
|--------|-------------|-------------|---------|-----------------|----------|-----------------|
| Neutral | 1.27 | 3.175 | 3.5 | 1.87 | 2.14×10\(^{-13}\) | 2.5 | 1.55 |
| Red    | 3.55 | 3.267 | 3.5 | 1.87 | 2.14×10\(^{-13}\) | 2.5 | 1.55 |

There is little variation in the position of peaks and the magnitude of the peaks is greater. A normal dispersion was observed at \(\lambda<500\) nm as well as anomalous dispersion at \(\lambda>500\) nm.

Based on the single-oscillator model (Wemple and Didomenico, 1971) is a semi-empirical dispersion relation for determining the refractive index \(n\) at photon energy \(h\nu\) can be written as follows Eq. 2:

\[
n^2 = 1 + \frac{E_o E_d}{E_o^2 - (h\nu)^2}
\]  

Where:

- \(h\) = The Planck constant
- \(\nu\) = The frequency
- \(E_o\) = the average excitation energy for electronic transitions
- \(E_d\) = The dispersion energy which is measure of the average strength of inter-band optical transitions or the oscillator strength

By plotting \((n^2-1)^{-1}\) against \((h\nu)^2\) and fitting a straight line as shown in Fig. 5 \((E_o E_d)^{-1}\) and the intercept \((E_o/E_d)\), on the vertical axis.

The long wavelength refractive index \((n_\infty)\) and average oscillator wavelength \((\lambda_0)\) and oscillator length strength \(S_0\) parameters for the NR can be determined by the single oscillator model given by Eq. 3 (Abdelmoneim, 2010):

\[
\frac{n_\infty^2 - 1}{n^2 - 1} = 1 - \left(\frac{\lambda_0}{\lambda}\right)^2
\]  

Dielectric constant: Once the dielectric function is known, it may be used to study the optical properties of the material studied. The dielectric constant can be defined as \(\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)\) and real and imaginary parts of the dielectric constant are related to \(n\) and \(k\) values and these values were calculated using the formulas Eq. 6 (El-Korashy et al., 2003; Wakkad et al., 2000):

\[
\varepsilon_1(\omega) = n^2(\omega) - k^2(\omega), \varepsilon_2(\omega) = 2n(\omega)k(\omega)
\]  

The \(\varepsilon_1\) and \(\varepsilon_2\) values for the film were calculated using Eq.(6) and are shown in Fig. 6a and b. The real part of the dielectric constant of the 3-amino-7-dimethylamino-2-methyl phenazine (NR) is higher than that of the imaginary part.

The real part of the dielectric constant relates to dispersion, whereas dissipative rate of the electromagnetic wave in the dielectric medium is provided by imaginary part. The UV-visible spectra of 3-amino-7-dimethylamino-2-methyl phenazine (NR) show some intense bands which are at ranges of 250-450 and 550-800 nm. The intensity and position of peaks observed change by metal coordination.
CONCLUSION

Optical properties of the dye polymer film by 3-amino-7-dimethylamino-2-methyl phenazine (NR) doped in Polyvinylpyrrolidone PVP have been investigated to obtain the optical constants. The refractive index dispersion parameters, oscillator energy \( E_o \), dispersion energy \( E_a \), long wavelength refractive index \( n_\infty \) and oscillator length strength \( S_0 \) change by metal coordination. The optical moments \( M_{-1} \) and \( M_{-3} \) of NR were calculated. The real and imaginary parts of the thin film were calculated.

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