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# Dispersion parameters and optical constants of Schiff Base derivative thin film

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**ABSTRACT**

*A new schiff base derivative (ShBD) [2,2(biphenyl-4-4-diylbis(azan-1-yl-1-ylidene)bis(methan-1-yl-1-ylidene)diphenol] was synthesized, and their structure was characterized by FTIR and CHN. The thin films was prepared by cast method, and the structural investigations performed by means of X-ray diffraction (XRD) technique which showed the shape structure. The dispersion of the refractive index was discussed in terms of the Wemple-DiDomenico single oscillator model. The values of some important parameters of the studied films are determined, such as $E_o$, $E_d$, $\varepsilon_\infty$ and a simple relation is suggested to estimate the third-order optical nonlinear susceptibility $\chi^{(3)}$. The estimations of the corresponding $\chi^{(3)}$and $\varepsilon_\infty$ are ($1.02\times10^{-10}$esu), (4.12) respectively.*

**Keywords:** Schiff Base; Optical properties; Dispersion energy parameters

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## INTRODUCTION

The band structure of semiconductor materials (amorphous or crystalline) has attracted increasing interest in recent years. Optical absorption and photo conductivity investigation provided an extremely valuable insight in understanding the nature of their band structure, which is related to the transport behavior of the carriers[1].

Knowledge of optical constants of the materials (optical band gap and extinction coefficient) is vital to scrutinize the atomic structure, electronic band structure and electrical properties. The refractive index is an important optical parameter for the design of prisms, windows and optical fibers[2].The refractive index provides the information about the chemical bonding and electronic structure of the material. An accurate measurement of the optical constant can be easily performed on semi-organic crystals[3].

The study of the optical absorption in the solids provides essential information about the band structure and the energy gap in the crystalline and non-crystalline materials. Analysis of the absorption spectra in the lower energy part gives information about atomic vibrations while the higher energy part of the spectrum gives knowledge about the electronic states in the atom[4].

Generally speaking, organic materials with conjugated molecular systems possess large third-order nonlinear susceptibility and ultra-fast response as a result of delocalization of π-electrons[5].Thin films are extremely thermally stable and reasonably hard, but they are fragile. On the other hand organic materials have reasonable thermal stability and are tough, but are soft[6].

## MATERIALS AND METHODS

***Materials and procedures:***
Ortho hydroxybenzaldehyde and Diphenyldiamine were obtained from Fluka Co., methanol and ethanol solvents were obtained from Merck Co. The chemical structural of the (ShBD) are shown in Fig.1.

In round bottom flask (20 m mole) from orthohydroxybenzaldehyde was put and the appropriate diphenyldiamine(10m mole) in ethanol (30ml) are refluxed for 1 hr. The pale yellow precipitate which formed was removed by filtration, washed with methanol and purified by recrystallization and dried in a vacuum oven at 60°C, their melting point was 190°C.

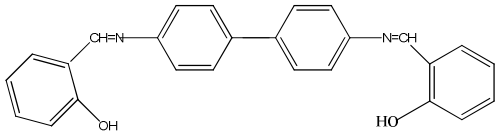



**Fig. 1 The chemical structure of the ShBD**

***Characterization:***
The FTIR spectra were obtained with a FT/IR-model 8400s spectrophotometer by Shimadzu, under ambient condition. Infrared spectroscopic studies were conducted to investigated the type of chemical bonding which illustrated in Fig. 2. The FTIR spectra of (ShBD) has fairly strong absorption in the region (1000-1600) $cm^{-1}$ and the bands in this region have contribution mainly from C=N (1569.95) $cm^{-1}$ stretch, C-N (1282.57) $cm^{-1}$ stretch, C-O (1184.21) $cm^{-1}$stretch, C=C (1618.17) $cm^{-1}$ stretch aromatic and C-H (2920.03) $cm^{-1}$ stretcharomatic bonds. Broad band were also observed at 3382.91 $cm^{-1}$ which is related to O-H group.

Elemental analysis of the (ShBD)was carried out using a Euro Vector EA 3000AItaly instrument, and which shown in Table 1.

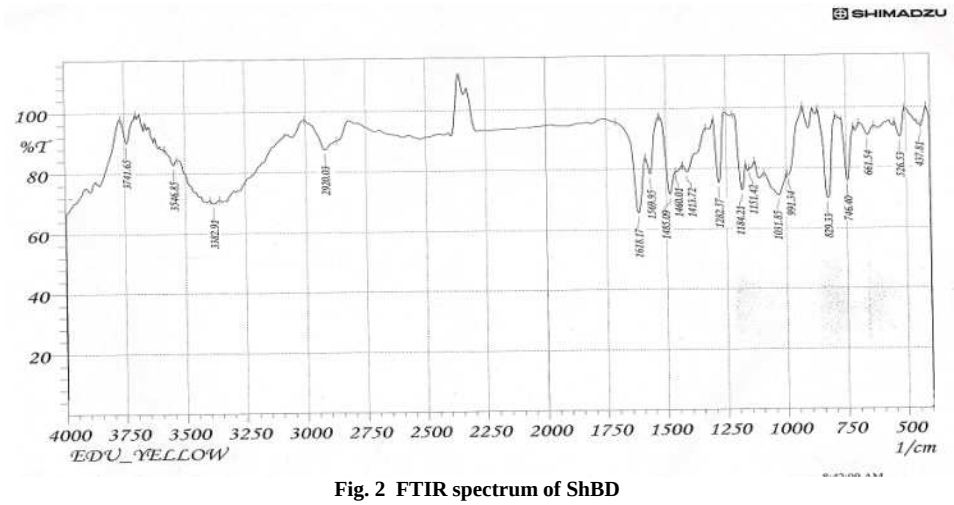



**Fig. 2 FTIR spectrum of ShBD**

**Table 1. Elemental analysis of functionalized ShBD**

| C% | | N% | | H% | |
|---|---|---|---|---|---|
| Theoretical | Calculated | Theoretical | Calculated | Theoretical | Calculated |
| 86.63 | 86.91 | 7.48 | 7.13 | 5.88 | 5.36 |

## RESULTS AND DISCUSSION

***Structural information of (ShBD):***
The X-ray diffraction (XRD) studies were carried out to get an idea about the structural changes produced in the investigated of (ShBD) thin films. The diffracted intensity as a function of the reflection angle was measured automatically by the X-ray diffractophotometer. The absence of a peak in X-ray spectra Fig. 3 confirmed the amorphous nature of (ShBD) sample.

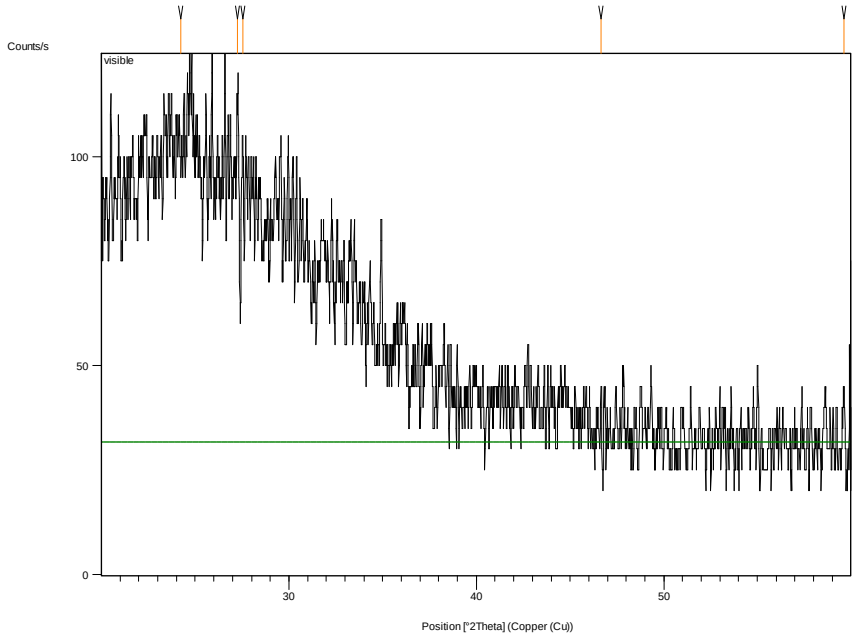



**Fig. 3 XRD chart of ShBD**

***Dispersion energy parameters of (ShBD) thin films:***

We determined values of *n* ( refractive index) and *k* (extinction coefficient) from the transmittance and reflectance spectra of the thin films. The reflectance spectra of thin films exhibit a peak at energies to the inter-band transitions. The extinction coefficient and refractive index of any solid certain constant wavelength are expressed as[7]:

$k = \frac{\propto \lambda}{4\pi}$(1)

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

The spectral curve of *n* value determined using above relationships as shown in Fig. 4.

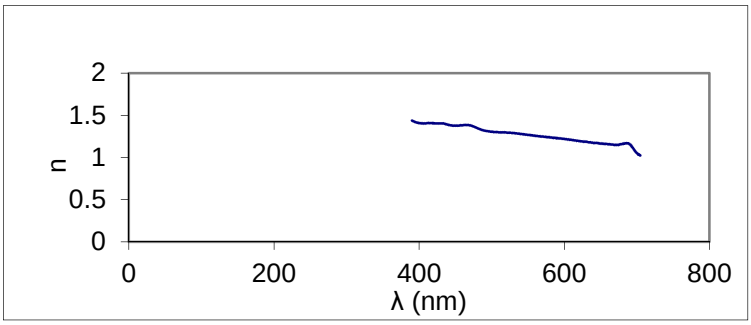



**Fig. 4 The refractive index plot of ShBD thin film**

Wimple and DiDomenico[8,9] use a single oscillator description of the frequency-dependent dielectric constant to define a *dispersion energy* parameter $E_d$ and $E_o$.The dispersion plays an important role in the research for optical materials, because it is a significant factor in optical communication and in designing devices for spectral dispersion. The relation between the refractive index *n* and the single-oscillator strength below the band gap is given by the expression[8,9].

$n^2 = 1 + \frac{E_0 E_d}{E_0^2 - (h\upsilon)^2}$(3)

Where $E_o$is the energy of the effective dispersion oscillator, $E_d$the so-called dispersion energy, which measures the average strength of inter band optical transitions.

Experimental verification of Eq.(3) can be obtained by plotting $(n^2\text{-}1)^{-1}$ versus$(h\upsilon)^2$as illustrated in Fig. 5.

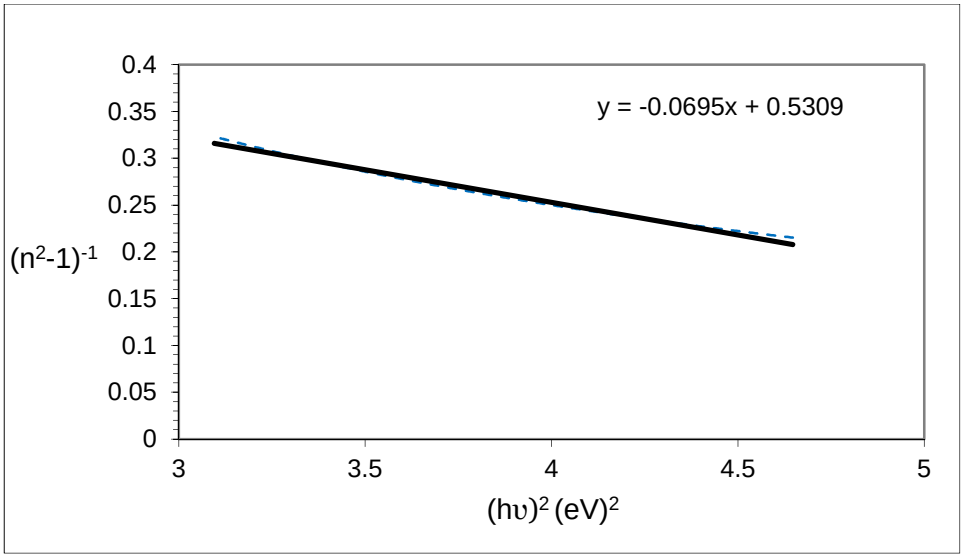



**Fig. 5 The plot of $1/(n^2\text{-}1)$ vs.( $(h\upsilon)^2$for ShBD thin film**

The dispersion parameters$E_o$and $E_d$ are described by means of the r[th] moment of the $\varepsilon_2(E)$ optical spectrum.

It is known that the r[th] moment of $\varepsilon_2(E)$ spectrum is defined as [10,11]:

$$M_r = \frac{2}{\pi}\int_{E_t}^{\infty} E_r\, \varepsilon_2(E)\, dE \quad (4)$$

Where E= hω and $E_t$ is the absorption threshold energy.

One can develop some relationships between the dispersion parameters and $\varepsilon_2(\omega)$ spectrum via:

$$E_o^2 = \frac{M_{-1}}{M_{-3}} \quad (5)$$

$$E_d^2 = \frac{M_{-1}^3}{M_{-3}} \quad (6)$$

Where $M_{-1}$, $M_{-3}$ are the moment of optical spectrum which are involved in computation of $E_o$and $E_d$. It is known that static dielectric constant of any substance is defined as:

$$\varepsilon_r(0) = \lim_{E\to 0} n^2(E) = n_o^2 \quad (7)$$

The static dielectric constant can be written in term of dispersion parameters simply as:

$$n_o^2 = \varepsilon_r(0) = 1 + \frac{E_d}{E_o} \quad (8)$$

The values of $E_o$, $E_d$, $M_{-1}$, $M_{-3}$ ,$n_o$, $\varepsilon_\infty$ are listed in Table 2.

**Table 2. The estimated values of the oscillator parameters of (ShBD) thin film**

| $E_o$(eV) | $E_d$(eV) | $n_o$ | $\varepsilon_\infty$ | $M_{-1}$ | $M_{-3}$ |
|---|---|---|---|---|---|
| 2.14 | 6.70 | 2.03 | 4.12 | 3.13 | 0.68 |

The long wavelength refractive index $n_\infty$, average inter band oscillator wavelength $\lambda_o$ and the average oscillator strength $S_o$ for the thin films were determined using the following relationship [12]:

$$\frac{(n_\infty^2-1)}{(n^2-1)} = 1 - \left(\frac{\lambda_o}{\lambda}\right)^2 \quad (9)$$

Where $n_\infty$ and $\lambda_o$ values were calculated from the plot of $(n^2\text{-}1)^{-1}$ vs. $\lambda^{-2}$ as shown in Fig. 6.

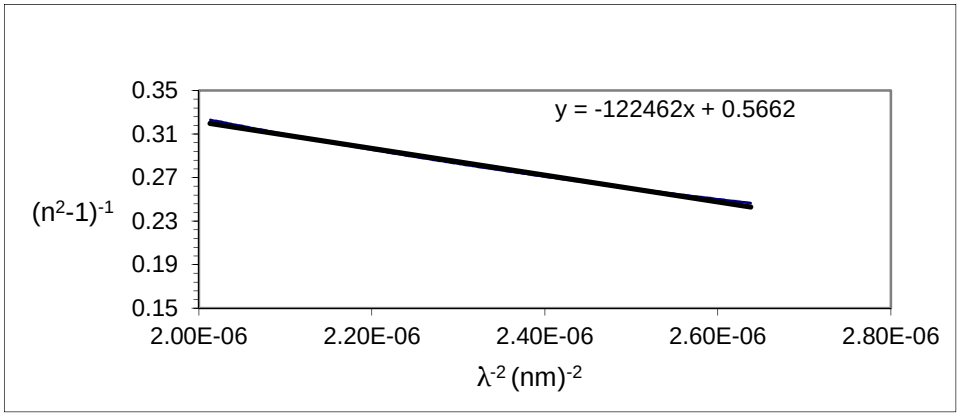



**Fig. 6 The $1/(n^2-1)$ vs. $\lambda^{-2}$ plot of ShBD thin film**

Eq.(9) can also be written as[13]:

$$n^2\text{-}1 = \frac{S_o \lambda_o^2}{(1-\lambda_o^2/\lambda^2)} \quad (10)$$

Where $S_o$ is the average oscillator strength which equals to:

$$S_o = \frac{n_o^2 - 1}{\lambda_o^2} \quad (11)$$

According toFrumar[14], the Miller rule is very convenient for visible, nonlinear and near infrared frequencies, which related the third order of nonlinear polarizability parameter $\chi^{(3)}$, the so-called nonlinear optical susceptibility, and the linear optical susceptibility $\chi^{(1)}$, through the equation:

$$\chi^{(3)} = A(\chi^{(1)})^4 = A\,[E_o E_d / 4\pi(E_o^2 - (h\upsilon)^2)] \quad (12)$$

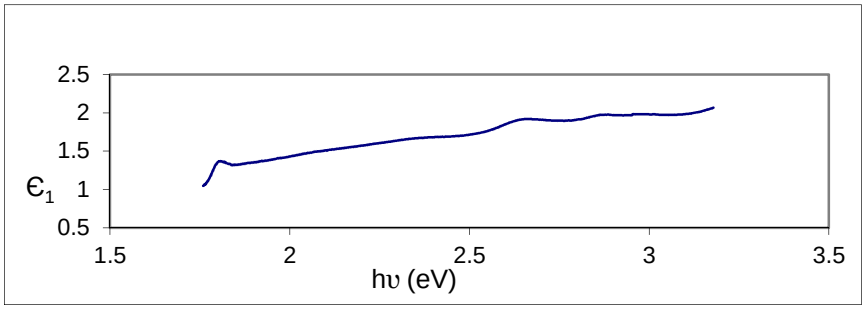
Where A is a constant, $A=1.7\times10^{-10}$.

The covalency and ionicity of the chemical bonds strongly influence the magnitude of the nonlinearity. The third-order nonlinear susceptibility of (ShBD) film is calculated by using Eq.(12).

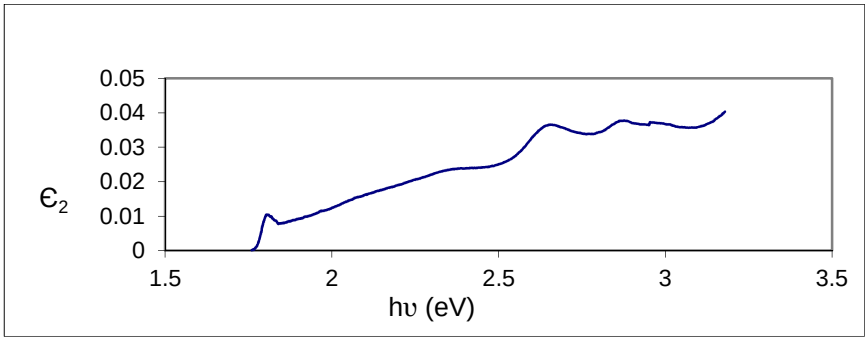
The real and imaginary parts of the dielectric constant can be given in the following form[15]:

$$\varepsilon_1 = n^2 - k^2 \quad \text{and} \quad \varepsilon_2 = 2nk \quad (13)$$

The dependences of $\varepsilon_1$and $\varepsilon_2$ on photon energy are shown in Fig. 7 (a,b).




**(a)**




**(b)**

**Fig. 7 The dielectric constant plot of (ShBD) thin film: (a) real part; (b) imaginary part**

The dissipation factor tan$\delta$ is a measure of loss-rate of power of a mechanical mode, such as an oscillation, in a dissipative system. The dissipation factor tan$\delta$ can be calculated to the following equation[16]:

$\tan\delta = \frac{\varepsilon_2}{\varepsilon_1}$(14)

The variation of dissipation factor of the investigation films with frequency F is shown in Fig. 8.

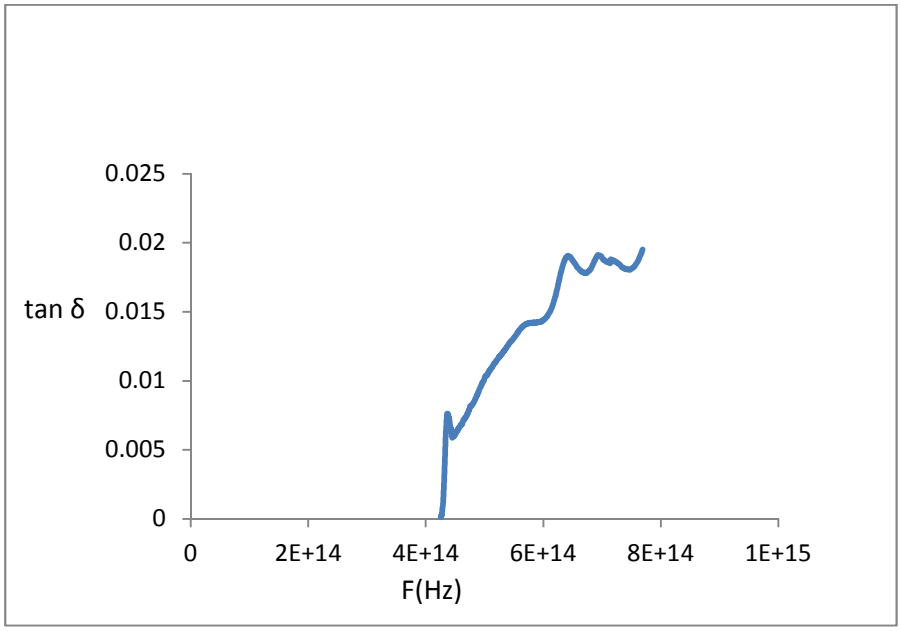



**Fig. 8 The variation of dissipation factor of the (ShBD) thin film**

It is found that the dissipation factor increases with increasing photon energy in the absorption region.

## CONCLUSION

In summary, schiff base derivative( ShBD) was synthesized and characterized. The thin film have been deposited on a glass substrate by cast method, and X-ray diffraction shows that it is an amorphous shape structure.

The dispersion of the refractive index in the thin film follows the single electronic oscillator mode. The values obtained for the oscillator strength ($E_d$) and the oscillator energy ($E_o$) are 6.70eV and 2.14eV respectively. The dielectric constant $\varepsilon_\infty$ is evaluated to 4.12, the third-order nonlinear susceptibility $\chi^{(3)}$ which is calculated using Frumar model, and it is estimated to be $1.02\times10^{-10}$esu.

The value of nonlinear optical susceptibility $\chi^{(3)}$indicated that new (ShBD) can be used widely in many photonic electronic applications.

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