



Determination and varying of of the optoelectronic parameters of 1, 4-Bis [2-(3-N-ethylcarbazoyl)-vinyl] benzene organic light emitting material (OLEM) with solvents

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Effects of solvents on optical properties of solutions of 1, 4-Bis [2-(3-N-ethylcarbazoyl)-vinyl] benzene (BCzVB) organic light emitting material (OLEM) have been studied by using solution method. The maximum mass extinction coefficient values of solutions of BCzVB material for DCM, THF, and chloroform solvents were determined to be 61.603, 51.295 and 22.647 Lg⁻¹cm⁻¹, respectively. The loss factor value for chloroform is the highest value, while the loss factor value for DCM solvent is the lowest value. The optical conductance values of the BCzVB are higher than the electrical conductance values of the BCzVB. It was found that the optical band gap value of the BCzVB material have increased by changing for various solvents. DCM, THF, and chloroform solvents were used to reach lower E_g values (2.815, 2.835 and 2.851, respectively).

Keywords: BCzVB; solvents, constant, optical/electrical conductance, VELF, SELF.

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1. Introduction

High flexibility, low power consumption, low thickness, and fast response [1] can be seen as some of the advantages of organic light emitting materials (OLEMs), have become a good candidate for industry of tablet computer, mobile phone and research institutes. To have full color at device applications- given a significant examples of high efficiency white organic light emitting diodes (WOLEDs) [2-7]. Blue and yellow or orange have given white-light emission, mixing of red, green and blue also have given white-light emission. It has been very clear that blue emitter [8-10] or dopants materials have become a key role in designing and understanding next generation OLEDs devices.

1, 4-Bis [2-(3-N-ethylcarbazoyl)-vinyl] benzene (BCzVB) material and its derivatives are vital materials for OLEDs. It was shown that additional BCzVBi dopants have become better optical and electrical properties of the blue OLEDs devices [11]. Research demonstrated that efficiency of luminous for device were %18 higher than those non additional BCzVBi dopant [11], underlying that blue emitter or dopants materials are of the prominent importance to control optical properties of the device. By using BCzVB and BCzVBi as a emitting layer materials, the maximum luminance 21 044 cd m² for driving voltage of 17 V with efficiency of maximum luminance 9.12 cd A⁻¹ can be obtained from WOLEDs having better in efficiency, color stability, and chromaticity [12].

Effects of solvents on UV spectra and on organics have been investigated for particularly last century [13]. These rely on mostly interactions of solvent-solute, of degree of dye-solvent and solvent nature [14,15]. BCzVB is soluble in known organic solvents given examples of tetrahydrofuran (THF), dichloromethane (DCM), and chloroform. By dissolving in THF, the solution of BCzVB was used as source materials to fabricate WOLEDs, having PL and absorption measurement given a better efficiency [16]. It has concluded that choice of solvents have effects on material's and device's optical and electrical properties.

Furthermore, several scientists have done a lot of researches on materials of BCzVB and its derivatives. Su-Hua Yang et al [17] reported that the measurement energy absorption of BCzVB greatly overlaps with 4, 40-bis (carbazol-9-yl) biphenyl (CBP) emission. It has concluded that blue dopant of BCzVB does a job as a medium and giving rise to an efficient emission of (C545T) [18]. It was not detected any research in the literature regarding optical properties of solutions of BCzVB material along with different solvents. Method of solution for researching of optical properties of soluble materials has a few merits such as lower cost and highly accurate outcomes. Taking into above considerations, it has been clear that studying the optical properties of solutions of BCzVB material plays a crucial role in understanding and improving next generation OLEDs and other devices and in opening up new applications areas.

In this research, optical properties of solutions of BCzVB material have been meticulously researched. The optical measurements have been performed by using Shimadzu model UV-1800 Spectrophotometer. The aim of the study was to explore effects of different solvents on optical and contrast properties. It was observed that values of optical band gap of BCzVB material solution were decreased with changing solvent.

2. Experimental

2.1. Having a prepare of BCzVB solutions

The 1, 4-Bis [2-(3-N-ethylcarbazoyl)-vinyl] benzene (BCzVB) organic light emitting material (OLEM) and solvents being chloroform, tetrahydrofuran (THF), and Dichloromethane (DCM) have been bought from Sigma-Aldrich Co, and all have been used in this research. Weightiness of BCzVB material has been measured by benefitting from an AND-GR-200 (10)

Series Analytical Balance for 0.0630 mM molarity. Soon afterward, it homogeneously has passed into solution of chloroform at 20 mL volume, 20 mL volume of THF, and 20 mL volume of DCM

solvents. To make sure to have homogeneously dissolved solutions, each sample was shaken for at least 20 minutes. At the final point, solutions of BCzVB material have been filtered by filter of PTFE membrane to make ready for having best outcome of optical measurement. Fig. 1 has displayed real pictures of top and side views of solutions of BCzVB material dissolved in different solvents. The aim of these processes is to examine effects of solvents on optical properties of BCzVB material.

2.2. Optical measurements of BCzVB solutions with different solvents

Length of optical path with 10 mm and (Hellma QS-100) cylindrical bathtub having 3.5 mL volume has been used for all solutions of BCzVB material to have accurate result. Before measurements, all equipment was chemically cleaned and then was thoroughly dried. Optical measurements for all solutions with different solvents were conducted, they were successfully documented by using UV-1800 Spectrophotometer (Shimadzu model) for wavelength 190-1100 nm with room temperature condition.

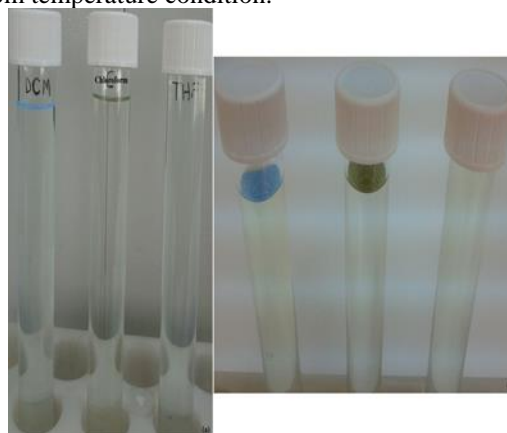


Fig. 1. The real pictures of top and side views of solutions of BCzVB material dissolved in different solvents.

3. Results and discussion

3.1. Effects on optical properties of BCzVB material with different solvents

Fig. 2 has exhibited the plot of absorption coefficient vs. energy of solutions of the BCzVB material with DCM, THF, and chloroform solvents. As shown in Fig 2, the absorption coefficient curves for DCM, THF, and chloroform solvents exhibit three peaks and the maximum peaks of BCzVB material for DCM, THF, and chloroform solvents occur at 3.148, 3.163 and 3.155 eV, respectively. The values of absorption coefficient of solutions of

BCzVB at maximum peaks with DCM, THF, and chloroform solvents are 2.005, 1.667 and 0.736 cm^{-1} , respectively. It has concluded that the value of absorption coefficient for DCM is the highest value, while the value of absorption coefficient for chloroform is the lowest value. It was seen that choice of solvent has an impact on absorbance parameter of solutions of the BCzVB material. Also, it has pointed out that the absorbance values of solutions of BCzVB material for different solvent lives in spectrum of about 230-450 nm covering near-ultraviolet, and some of visible region. The maximum absorption wavelength (λ_{max}) values of solutions of BCzVB material with DCM, THF, and chloroform solvents were determined to be 394, 392 and 393 nm, respectively. All these values have been lower than the maximum absorption values of 402 nm and 428 nm of BCzVB material referred to literature [16].

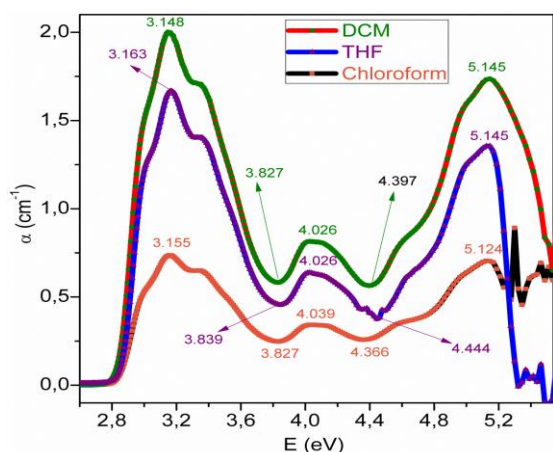
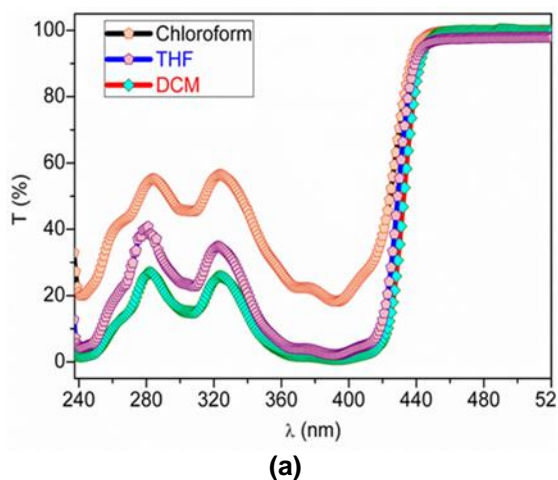
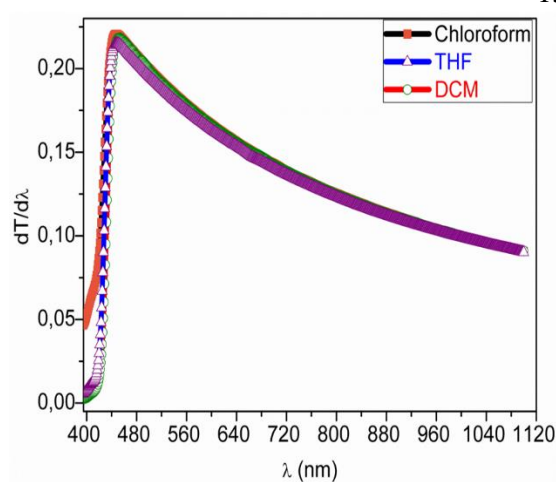


Fig. 2. The plot of absorption coefficient vs. energy of solutions of the BCzVB material with DCM, THF, and chloroform solvents.



(a)



(b)

Fig. 3. The (a) transmittance vs. λ and (b) $dT/d\lambda$ vs. λ plot of the solutions of the BCzVB material with DCM, THF, and chloroform solvents.

One of the significant optoelectronic parameters is the molar extinction coefficient (ϵ); many disciplines of chemical, engineering, scientific covering interactions of photo have needed to this parameter [19]. The maximum molar extinction coefficient (ϵ_{max}) values of solutions of BCzVB material with DCM, THF, and chloroform solvents were determined to be 31.828×10^3 , 26.502×10^3 and $11.701 \times 10^3 \text{ Lmol}^{-1}\text{cm}^{-1}$, respectively. These ϵ_{max} values have been lower than the value ($193.1 \times 10^3 \text{ Lmol}^{-1}\text{cm}^{-1}$) of solutions of TDCV-TPA [20] referred to literature. Value of molar extinction coefficient for DCM has been higher than that of THF, and value of molar extinction coefficient for THF is higher than that of chloroform. The maximum mass extinction coefficient ($\epsilon_{\text{max-mass}}$) values of solutions of BCzVB for DCM, THF, and chloroform solvents were determined to be 61.603, 51.295 and $22.647 \text{ Lg}^{-1}\text{cm}^{-1}$, respectively. It has suggested that choice of solvent for BCzVB material has affected the value of maximum mass extinction coefficient.

Fig 3a shows plot of transmittance (T) versus wavelength of the solutions of the BCzVB with DCM, THF, and chloroform solvent. The T values for chloroform solvent are the highest values, while the T values for DCM solvent are the lowest values. It has concluded that solvents have an important role on transmittance spectra of BCzVB material. Fig 3b was plotted to have values of absorption band edge of solutions of BCzVB material and it shows the figure of $dT/d\lambda$ versus λ of solutions of BCzVB with DCM, THF, and chloroform solvents. The absorption band edge values of solutions of BCzVB material for DCM, THF, and chloroform solvents were determined to be 2.737, 2.768 and 2.774 eV, respectively. All

absorption band edge values of BCzVB material for DCM, THF, and chloroform solvents have been higher than values (from 2.195 eV to 2.206 eV) PTCDI-C5 molecule [21] referred to literature. It has suggested that the absorption band edge value for chloroform is the highest value, while the absorption band edge value for DCM is the lowest value.

Optical band gap (E_g) of optical transitions has been computed by benefitting from well-known relation, Tauc relation [22];

$$(\alpha h\nu)^n = C(h\nu - E_g) \quad (1)$$

where $h\nu$ denotes photon energy, n denotes parameter measuring type of band gaps, C denotes constant and E_g denotes optical band gap of used material. Fig. 4 shows $(\alpha h\nu)^2$ plot versus photon energy (E) of BCzVB material for DCM, THF, and chloroform solvents. The E_g values of solutions of BCzVB material were obtained from Fig. 4. The E_g values of solutions of BCzVB for DCM, THF, and chloroform solvents are found to be 2.815, 2.835 and 2.851 eV, respectively. These results suggest that the E_g value for chloroform is the highest value, while the E_g value for DCM is the lowest value. It was revealed that solvents have a significant impact on optical band gap, is of the prominent importance to optoelectronic, and photonic devices.

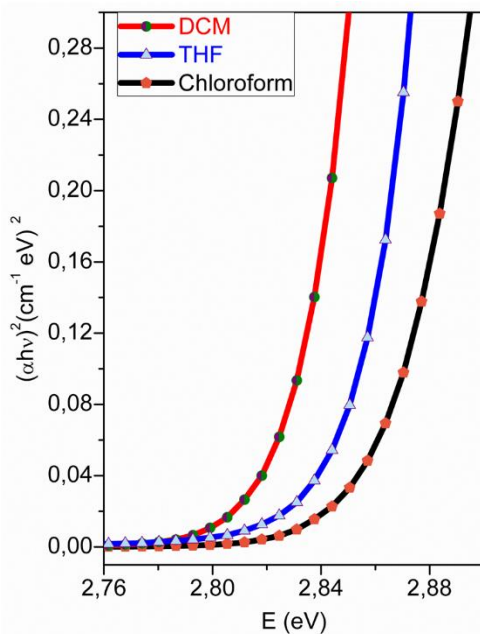


Fig. 4. The $(\alpha h\nu)^2$ plot vs. the photon energy (E) of the BCzVB material with DCM, THF, and chloroform solvents

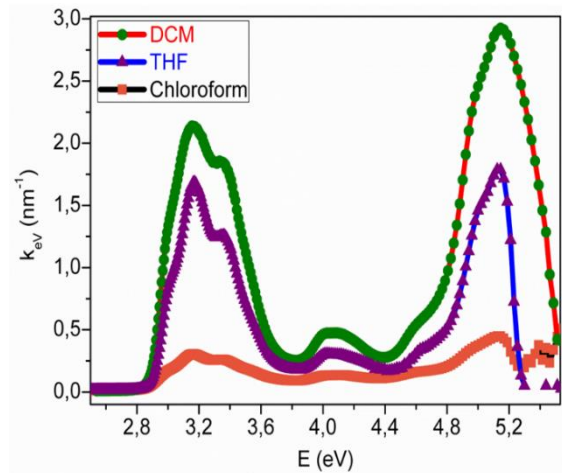


Fig. 5. The propagation constant (k_{ev}) plot vs. E of the BCzVB material with DCM, THF, and chloroform solvents

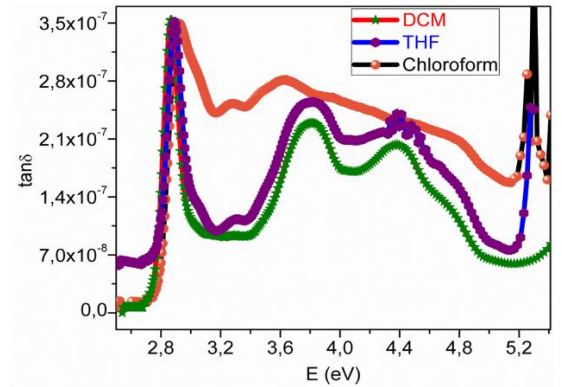


Fig. 6. The loss factor ($\tan\delta$) vs. E of the BCzVB material with DCM, THF, and chloroform solvents

Propagation constant (k_{ev}) is expressed as [21]

$$k_{ev} = \frac{2\pi}{\lambda} n_2 \sin\theta_1$$

The k_{ev} values of the BCzVB material for different solvents were calculated from Eq. (2) and the plot of the k_{ev} vs. E of the BCzVB for DCM, THF, and chloroform solvents is shown in Fig.

5. As seen in Fig. 5, the propagation constant value of BCzVB material for DCM, THF, and chloroform solvents varies from about 0 to 2.95 nm^{-1} . The k_{ev} value for DCM is the highest value, while the k_{ev} value for chloroform is the lowest value.

The loss factor ($\tan\delta$) is evaluated by [21,23];

$$\tan \delta = \frac{\epsilon_2}{\epsilon_1} \quad (3)$$

The $\tan\delta$ values of the BCzVB for DCM, THF, and chloroform solvents were computed from Eq. (3). The plot of the $\tan\delta$ as a function of E of the BCzVB for DCM, THF, and chloroform solvents is shown in Fig. 6. As seen in Fig. 6, the $\tan\delta$ values of the BCzVB material are almost constant until about 2.65 eV, then they sharply increases and have highest peaks (at about 2.88 eV). Obtained results show that the $\tan\delta$ value for chloroform is the highest value, while the $\tan\delta$ value for DCM solvent is the lowest value.

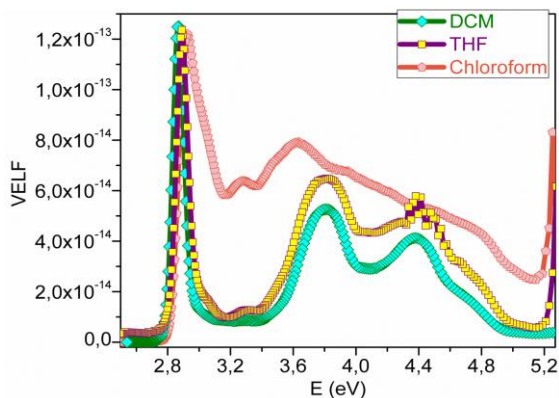
The volume and surface energy loss functions (VELF and SELF) are dispersion parameters and they are related to dielectric constants. The VELF and SELF can be determined by [23,24]:

$$VELF = \frac{\epsilon_2^2}{(\epsilon_1^2 - \epsilon_2^2)} \quad (4)$$

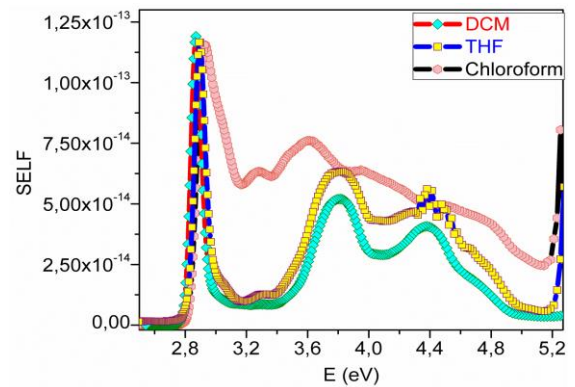
and

$$SELF = \frac{\epsilon_2^2}{((\epsilon_1 + 1)^2 + \epsilon_2^2)} \quad (5)$$

The VELF and SELF values of the BCzVB for DCM, THF, and chloroform solvents were calculated from Eq. (4) and (5), respectively. Fig. 7(a,b) indicates the curve of the VELF and SELF as a function of E for BCzVB material. As seen in Fig. 7(a,b), VELF and SELF values of the BCzVB material are almost the same for DCM, THF, and chloroform solvents. As seen in Fig. 7(a,b), the VELF and SELF values of the BCzVB material for chloroform are the highest values, while the VELF and SELF values for DCM solvent are the lowest values.



(a)



(b)

Fig. 7. The (a) volume energy loss function (VELF) and (b) surface energy loss function (SELF) vs. E of the BCzVB material with DCM, THF, and chloroform solvents.

3.2. The contrast properties of the BCzVB material for different solvents

Contrast (α_c) of a material can be obtained by [25-26];

$$\alpha_c = 1 - \left(\frac{n_1}{n_2} \right)^2 \quad (6)$$

In Fig. 8, it was given the figure of the contrast (α_c) versus E of BCzVB material for DCM, THF, and chloroform solvents. Fig. 8 has exhibited the α_c versus E of solutions of BCzVB for DCM, THF, and chloroform solvents. The contrasts of the BCzVB for DCM, THF, and chloroform solvents have increased with increasing photon energy. Contrasts of BCzVB material keenly increase starting point about 2.65 eV up to about 2.90 eV.

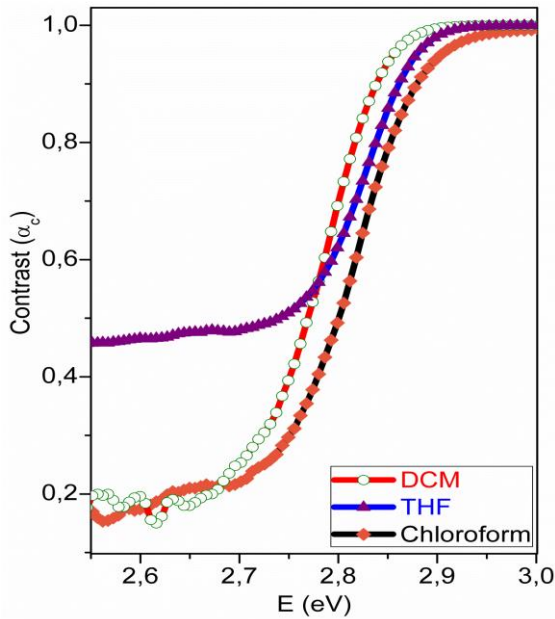


Fig. 8. The contrast (α_c) vs. E of the solutions of the BCzVB material with DCM, THF, and chloroform solvents

3.3. Comparison of the optical and electrical conductance

The optical conductance (σ_{op}) and electrical conductance (σ_{elec}) of the materials can be calculated using the formula [27]

$$\sigma_{op} = \frac{\alpha nc}{4\pi} \quad (7)$$

and

$$\sigma_{elec} = \frac{2\lambda\sigma_{op}}{\alpha} \quad (8)$$

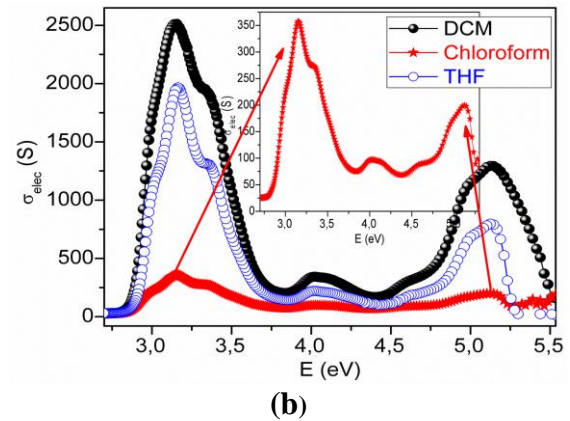
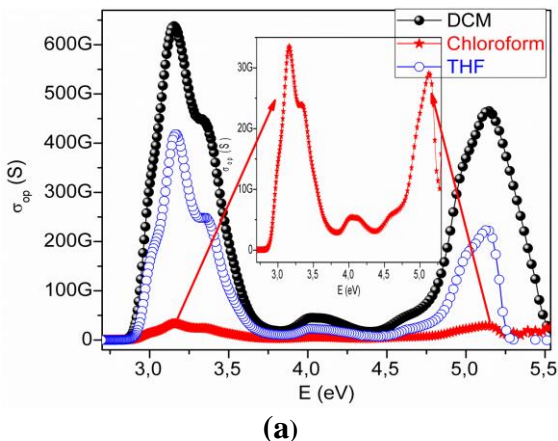


Fig. 9. The optical conductance (σ_{op}) and electrical conductance (σ_{elec}) plot vs. E of the solutions of the BCzVB material with DCM, THF, and chloroform solvents.

where c is the velocity of light. Fig. 9(a,b) indicates the σ_{op} and σ_{elec} plot vs. E of the BCzVB material, respectively. As seen in Fig. 9(a,b) and its inset, the σ_{op} and σ_{elec} values of the BCzVB material for DCM, THF and chloroform solvents in the same molarity are different from each other. Also, the σ_{op} and σ_{elec} curves exhibit two prominent peaks for DCM, THF and chloroform solvents and these peaks and their σ_{op} and σ_{elec} values are given in Table 1. As seen in Table 1, the first prominent σ_{op} peaks for DCM, THF and chloroform solvents are observed at 3.155, 3.164 and 3.163 eV, while the first prominent σ_{elec} peaks for DCM, THF and chloroform solvents are observed at 3.155, 3.164 and 3.155 eV, respectively. This result suggests that the first prominent σ_{op} and σ_{elec} peaks for chloroform solvent occur at different wavelengths (at 3.163 and 3.155 eV, respectively), while the first prominent σ_{op} and σ_{elec} peaks for DCM and THF solvents occur at the same wavelengths (at 3.155 and 3.164 eV, respectively). On the other hand, as seen in Table 1 the second prominent σ_{op} peaks for DCM, THF and chloroform solvents are observed at 5.145, 5.124 and 5.124 eV, while the second prominent σ_{elec} peaks for DCM, THF and chloroform solvents are observed at 5.124 eV. This result suggests that the second prominent σ_{op} and σ_{elec} peaks for DCM solvent occur at different wavelengths (at 5.145 and 5.124 eV, respectively), while the second prominent σ_{op} and σ_{elec} peaks for THF and chloroform solvents occur at the same wavelengths (at 5.124 eV).

Obtained results show that the σ_{op} and σ_{elec} values of the BCzVB material for DCM solvent are the highest, while the σ_{op} and σ_{elec} values of the BCzVB material for chloroform solvent are the lowest. In addition, the optical conductance values of the BCzVB are higher than the electrical

conductance values of the BCzVB. The optical and electrical conductance values of the BCzVB tend to increase at the related peaks. This increase can be attributed to increase in the absorption coefficient in this region

Table 1. The optical conductance (σ_{op}) and electrical conductance (σ_{elec}) parameters of the BCzVB material for DCM, THF, and chloroform solvents.

Solvents	Sol	σ_{op}	σ_{elec}	σ_{op}	σ_{elec}
		(S)	(S)	(S)	(S)
Di chloromethane (DCM)	DCM	0.155	0.380	0.145	0.654
		0.164	0.181	0.124	0.230
		0.163	0.335	0.124	0.290
Tetrahydrofuran (THF)	THF	0.155	0.512	0.124	0.293
		0.164	0.966	0.124	0.797
		0.155	0.357	0.124	0.199

4. Conclusions

In this study, effects of solvents on optical properties of 1, 4-Bis [2-(3-*N*-ethylcarbazoyl)-vinyl] benzene (BCzVB) has been elaborately investigated by using the solution technique being cheaper and available to have high accurate results comparing to film technique. It was found that the optical band gap-powerful parameter for optoelectronic devices-of the solutionof the BCzVB material have increased with changing for various solvents. The transmittance values of solutions of BCzVB material for different solvents were determined in visible region, and can be applicable to some devices such as image sensor packaging structure.

The maximum molar extinction coefficient (ϵ_{max}) values of solutions of BCzVB material with DCM, THF, and chloroform solvents were determined to be 31.828×10^3 , 26.502×10^3 and 11.701×10^3 $Lmol^{-1}cm^{-1}$, respectively. The propagation constant value for DCM is the highest value, while the propagation constant value for chloroform is the lowest value. For future perspective, researching optical properties of BCzVB material have major impact on improving and comprehending next generation OLEDs and other devices; and then it has opened up original and industrial applications areas.

Acknowledgments

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