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Optoelectronic parameters of TBADN organic molecule: New aspect to solution technique

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ABSTRACT

2-tert-Butyl-9,10-di(naphth-2-yl)anthracene (TBADN) molecule have enormous applications in organic light-emitting diodes (OLEDs), transistors and organic lasers. These applications are based on its spectral, sensing and optical properties. The important spectral and sensing parameters of TBADN were calculated. The optical band gap values of TBADN were found to be 2.834, 2.775 and 2.674 eV for molarities of 0.3, 0.9 and 2.7 mM, while the optical band gap values of the TBADN for 0.25 mM of chloroform, DCM and THF solvents are 2.892, 2.904 and 2.930 eV, respectively. Impacts on the molarities and solvents on optical properties were investigated. In order to obtain lower optical energy gap of the TBADN, chloroform solvents can be preferred, while THF as a solvent can be preferred in applications of the TBADN molecule-based optoelectronic devices due to its higher transmittance spectrum.

1. Introduction

The term “organic semiconductor” is used to describe organic materials which have the capable of movement of electrons. They have fascinated great interest, since the exploration of these systems has produced a completely new concepts in scientific area [1]. They consist of a broaden electron system which can be altered in terms of conducting electrons. These semiconductors are divided into small molecules and higher molecular weight polymeric semiconductors. Small molecule organic semiconducting materials have some abilities such as, low cost, flexibility and applicability to slight optoelectronic devices, so they can be considered as useful materials in organic light-emitting diodes (OLEDs) [2], transistors [3] and organic lasers [4]. Anthracene and derivatives are members of the small organic molecules and they have significant effects on several semiconducting and photonic applications.2-*tert*-Butyl-9,10-di(naphth-2-yl)anthracene (TBADN) molecule studied in this research is one of the anthracene derivatives.

Many researchers reported the many studies on anthracene and its derivatives, especially TBADN material being used as a single molecule or mixed it with different materials. Jarikov et al. [5] studied the degradation mechanism and electron current of bipolar and unipolar devices included TBADN molecule. Khan et al. [6] used the TBADN material as a layer building several devices in order to find the efficiency, current density and luminance properties of those devices. Wei et al. [7] demonstrated the efficiency of white organic light emitting diodes with their good performances based on the luminance properties of the TBADN film includes different layers with other materials. Mao et al. [8] investigated the characteristics of solution technique and vacuum processed devices of different films which consist of TBADN material as a layer. TBADN molecule have been also studied as a layer for organic light-emitting applications due to its better device efficiencies [9–17]. Hsieh et al. [18] investigated the electrical properties and diffusion mechanism of anthracene derivatives molecule using admittance spectroscopy. Luo et al. [19] studied changes in photoluminescence yield of TBADN as a blue emitter in organic light emitting devices. Lee et al. [20] studied the effect of solvents on the structure of the solution-processed films. They [20] dissolved 5 wt% (DPAVBi): 95 wt% 2-(t-butyl)-9,10-bis(20-naphthyl) anthracene (TBADN) in toluene and chlorobenzene. Feng et al. [21] have comparative study of organic small molecules includes TBADN film prepared by solution and vacuum deposition based on different parameters.

In this study, we investigated in detail spectral, sensing and optical properties of solutions of the TBADN molecule for different molarities and solvents. The optical measurements were taken with a Shimadzu model UV–1800 Spectrophotometer. The spectral, sensing and optical parameters were obtained, controlled and advanced with different molarities and solvents.

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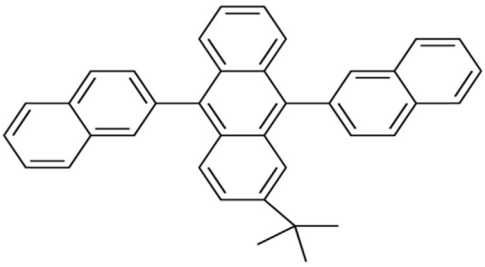

Fig. 1. The chemical representation of the 2-*tert*-Butyl-9,10-di(naphth-2-yl)anthracene (TBADN) molecule.

2. Experimental procedure

2-*tert*-Butyl-9,10-di(naphth-2-yl)anthracene (TBADN) organic molecule, chloroform, dichloromethane (DCM) and tetrahydrofuran (THF) solvents were used in this research. The chemical representation of the TBADN molecule is shown in Fig. 1. First, we prepared the solutions of the TBADN for various molarities and solvents. Secondly, we recorded the spectral and optical measurements of the solutions of the TBADN for different molarities and solvents.

2.1. Preparation of the solution of the TBADN different molarities and solvents

The molecular weight and formula of the TBADN molecule is 486,64 g/mol and $C_{38}H_{30}$, respectively. To prepare the solutions, TBADN materials were weighed with a AND-GR-200 Series Analytical Balance for different molarities (0.3, 0.9 and 2.7 mM) and dissolved homogeneously in 10 mL volume of THF solvent. Similarly, the weighed TBADN materials for 0.25 mM of different solvents (chloroform, DCM and THF) were dissolved homogeneously in 10 mL volume of the related solvents.

2.2. The UV measurements for different molarities and solvents

Length of optical path with 10 mm and (Hellma QS-100) cylindrical bathtub having 3.5 mL volume were used for all the solutions of the TBADN. The UV measurements of the TBADN molecule for different molarities and solvents were taken with a Shimadzu model UV-1800 Spectrophotometer in the wavelength 1100–190 nm at room temperature.

3. Results and discussion

Spectral properties of the TBADN organic molecule were firstly investigated. Then, we investigated in depth the optical properties of the solutions of the TBADN for 0.3, 0.9 and 2.7 mM of the molarities. The impacts of the molarity on the optical parameters were investigated. Finally, we investigated in depth the optical properties of the solutions of the TBADN for 0.25 mM of the different solvents (chloroform, DCM and THF). The impacts of the solvents on the optical parameters were additionally explored.

3.1. The impacts of the various molarities on properties of the solutions of the TBADN

Absorbance is the measurement of the amount of light absorbed. The absorbance spectra of the TBADN molecule were performed to look into their optical properties for different molarities. As viewed in Fig. 2, the absorbance values of the TBADN are dominant in the near ultraviolet (NUV) region. This indicates that the near ultraviolet region is critical for the TBADN molecule. We can see from the Fig. 2, the absorbance value diminishes definitely after 395 nm. For 2.7 mM, there is a peak at 248 nm, yet after that value the uncertainty shows

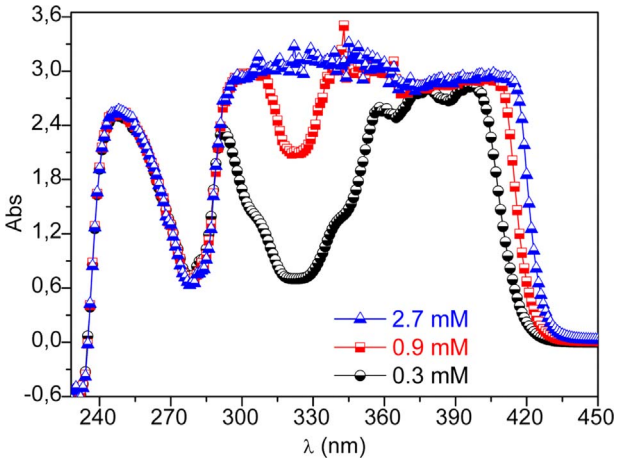

Fig. 2. The plot of the absorbance as a function of λ of the TBADN molecule for different molarities.

up. It is clear from the Fig. 2. that the absorbance of the TBADN increases with increasing molarity. Notwithstanding what has been said, the sensitivity of the TBADN molecule can be changed by different molarities. Tao et al. [22] synthesized the TBADN films for OLEDs. They [22] investigated the absorbance spectra of TBADN film and solution in DCM solvent. Diao et al. [23] characterized TBADN small molecule organic dye nanoparticles in tetrahydrofuran solution and investigated the UV–vis absorption of nanoparticles and solution of TBADN.

Absorption occurs when the energy is absorbed by an electron resulting in a transition from ground state to an excited state. The variation of spectral absorption coefficient (α) as a function of photon energy (hυ) of the TBADN molecule at different molarities is shown in Fig. 3. All the absorption maxima values of the TBADN for 0.3 mM are observed as seen in Fig. 3. It is also evident from the figure that there are two peaks for absorption maxima values of a TBADN molecule for 0.9 mM and there is just one peak for 2.7 mM. Also, the absorption bands of TBADN have five peaks at 3.13, 3.27, 3.46, 4.24 and 5.00 eV for 0.3 mM. Since in the NUV region there are four peaks, electronic range of TBADN can be referred to π–π* transition which is the generally essential and useful transition in UV spectroscopy [24]. This transition fall in an experimentally convenient region of the spectrum. Besides, the B-band or Soret results from near ultraviolet. It is obvious from the figure that there is an increment for absorption coefficients of TBADN molecule with the increase in molarities.

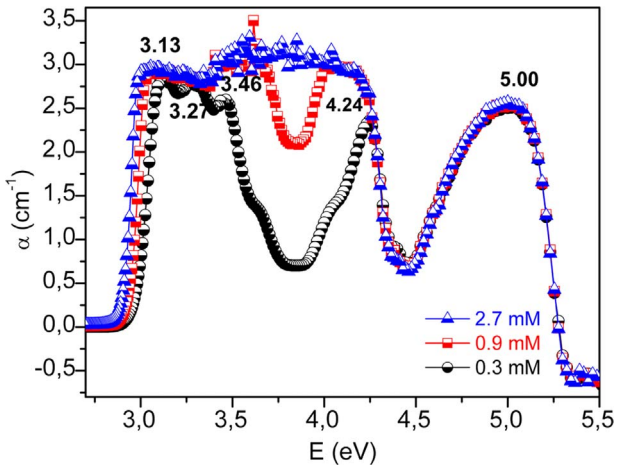

Fig. 3. The plot of the absorption coefficient (α) versus photon energy (hυ) of the TBADN molecule for different molarities.