OLED Display Application of 2-(6-Fluoro-2-oxo-2H-chromen-4-ylmethoxy)-benzoic Acid Methyl ester Derivative

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Abstract. White light emitting diodes (WLED) has received much importance due to their vast applications in various sensors, lightning devices and display etc. By mixing certain amount of green, red and blue, white light can have produced. Therefore, we made an attempt to produce a LED application device making use of organic compounds. Hence, we synthesized 2-(6-Fluoro-2-oxo-2H-chromen-4-ylmethoxy)-benzoic acid methyl ester (2–FBME) coumarin. In this present work the band gap energy is calculated and the photoluminescence spectra of 2–FBME molecule is studied in different solvents, this result shows the compound can be used to produce the desired wavelength. Hence,2–FBME possesses high color purity, good CIE chromaticity coordinate, and they would have potential organic light emitting devices (OLED) application, this simple method is used to produce the blue light as blue component can play important role in WLED.

INTRODUCTION

Among various derivatives of coumarins, benzopyrane derivatives have drawn much importance since they are well-known to possess distinct pharmacological and biological properties viz., antifungal, anti-HIV, antibiotic, antiviral, antibacterial, anticoagulant, anticlotting and anticancer and also proved several applications in different fields. The coumarins and their derivatives were privileged oxygen heterocyclic compounds occurred in several natural products. Further, the novel benzopyrane derivatives has fascinated the scientific community due to the interesting applications of synthesized compounds such as red and green OLEDs have met the requirements for practical applications. The literature revealed that, the different kinds of methods have been developed for the synthesis of biologically and spectroscopically active benzopyrane derivatives, specially the catalytic method[1-2]. Therefore, we attempted to synthesis 2-(6-Fluoro-2-oxo-2H-chromen-4-ylmethoxy)-benzoic acid methyl ester (2–FBME) dye using acetic acid as a catalyst. Furthermore, the electronic spectra of 2–FBME derivative in solutions depending on the solvents parameters they showed excellent fluorescence properties. These derivatives also exhibit the phenomena such as inter molecular charge transfer (ICT) and excited state intermolecular proton transfer which were played a major role in view of excellent photophysical properties like large stoke shifts, significant photostability and intense luminescence[3]. However, in literature there is no considerable report on the fluorescence studies of 2–FBME coumarin compound. To this end, the present paper reports on the fluorescence properties, Commission Internationale de I'Eclairage (CIE) and color purity of previously mentioned compound in different solvents.

EXPERIMENTAL

Synthesis Procedure and Materials used

The spectroscopic grade solvents such as Chloroform, Cyclohexane, Ethanol, Butanol, Decanol, Methanol and Propanol were purchased from the local chemical supplier having 99.9% purity were used without purification. The

UV-Vis absorption spectra of 2-FBMEwas recorded using UV-1800 Shimadzu spectrophotometer from 200-800 nm wavelength range. Steady-state fluorescence experiment was carried out making use of Hitachi F-2700 Fluorescence Spectrofluorometer. The selected excitation wavelength is used for recording the fluorescence emission and obtained more resolution at the highest intensity. The experiment (all measurements) were carried out at 274 Kelvin with solution concentration of 10^{-6}–10^{-7} M to overcome inner filter effect and self-aggregation effect. The detailed synthesis procedure and method carried out is mentioned in our previous report[1].

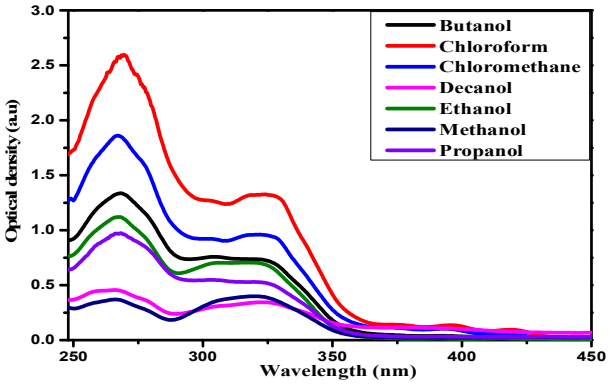


FIGURE1. The UV-Vis absorption spectra of 4-FBME in selected solvents

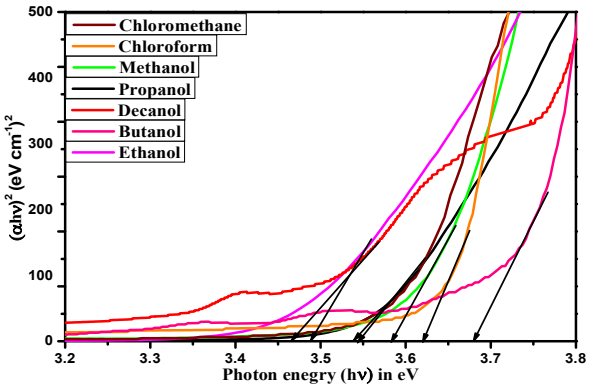


FIGURE2. Typical plot of $(\alpha h\nu)^2$ versus Photon energy for direct band gap measurements.

RESULTS AND DISCUSSION

We have studied theUV-Vis absorption spectra Fig. 1. and determined the band gap energy of the titled molecule by experimentally and theoretically. The plots of (αhν)2 versus photon energy hν for solutions of titled compound is depicted in Fig. 2, energy band gap Eg is determined and the values are presented in Table 1. However, the Eg is also calculated theoretically by using Gaussian 09 software (B3LYP-6-311G basic set) which is found to be 3.62 eV[4].The molecular orbital HOMO and LUMO energy figure is dissipated in Fig. 3.from this studies, we can conclude that the Eg experimentally and theoretically are same values. The photoluminescence (PL) emission spectra of the synthesized 2-FBME coumarin derivative in different organic solvents of varying dielectric constant and refractive index such as Chloroform, Cyclohexane, Ethanol, Butanol, Decanol, Methanol and Propanol.The PL spectra of synthesized2-FBME presented in Fig. 4. The sample was excited at 280 nm wavelength and the corresponding PL spectra shows the three emission peaks observed in all the studied solvents. In case of Chloromethane and Chloroform, the emission peaks are obtained at 405, 430 and 453 nm and in case of alcohols (used in this study) the emission peaks are observed in range between 406 to 568 nm. These observed behavior clearly indicates the influence of specific interactions in between solute and solvent used in the study, beyond that, from Fig. 4, the emission spectra showed a slight bathochromic shift (red shift) in all studied solvents, these shifts are probably due to increase in the polarity of the solvents indicates $\pi \rightarrow \pi^*$ transitions are involved[4,5].Also suggesting that the involvement of photo induced intermolecular charge transfer (ICT) state apart from solvent polarity, the hydrogen bonding effect also plays a major role for the shift of emission bands. And also the observed phenomenon i.e., duality nature of wavelengths in 2-FBME molecule in different solvents is due to solvation effect, this results shows a simple extraction of dye in different solvents can be used to produce the desired wavelength[5].

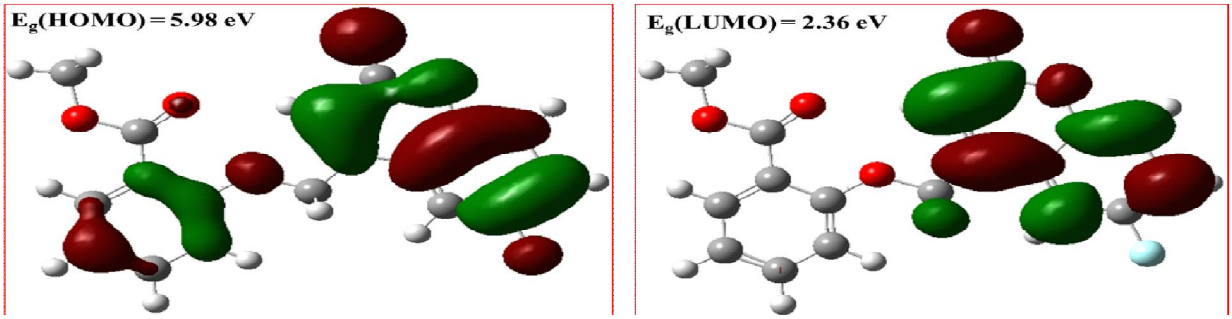
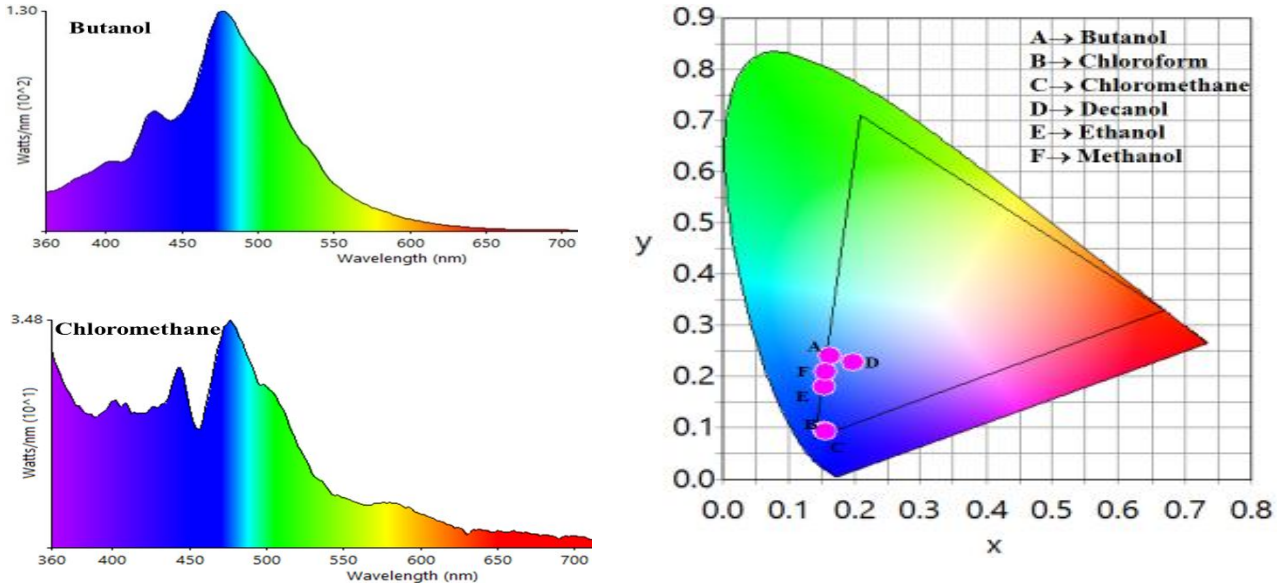


FIGURE 3. The molecular orbital structure (HOMO and LUMO) of 2-FBME in ground state.

The Commission Internationale de l'Eclairage (CIE) color coordinate values has been determined by using Osram Sylvania CIE co-ordinates software[6]. From the Fig 4 it is clear that the CIE coordinates lies in deep blue region for Chloroform, Cyclohexane, Ethanol, Butanol, Decanol, Methanol and Propanol the corresponding x and y values are tabulated in Table 1. The color purity is an important property to estimate the possibility of the newly synthesized 2-FBME derivative for OLEDs and display applications[7]. The color purity of the 2-FBME is calculated using the following equation

$$\text{Color purity} = \frac{\sqrt{(X - X_i)^2 + (Y - Y_i)^2}}{\sqrt{(X_d - X_i)^2 + (Y_d - Y_i)^2}} \text{ x } 100\%$$

However, this results revealed that the observed the color coordinates of 4-FBME slightly vary with different solvents due to decrease in intensity as well as the area of the photoluminescence emission. Thus, the 2-FBME possesses high color purity and good CIE chromaticity coordinate also they would have potential application of organic light emitting devices, this simple method is to produce the blue light as blue component can play important role. The calculated chromaticity coordinates for 2-FBME in chloroform are near to standard chromaticity (NTSC) for excellent blue color and thus are promising blue producers for WLED application[8-10].



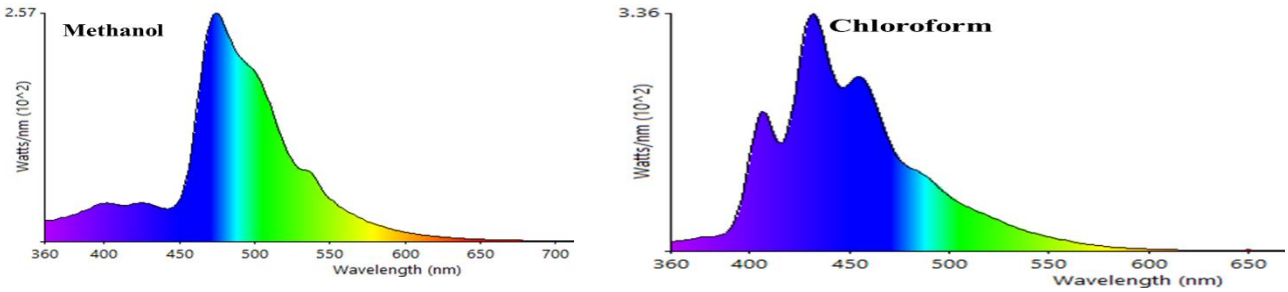


FIGURE 4. PL emission spectra of Butanol, Chloromethane, Methanol and Chloroform solvents with CIE Plots of 2-FBME molecule.

Where, (X, Y) are CIE chromaticity coordinate values of studied compound, (Xi, Yi) is the color coordinate of white illumination and (Xd, Yd) is the CIE coordinate of the dominant emission wavelength. In this report the (Xi, Yi) = (0.310, 0.316), (Xd, Xd) = (0.14, 0.08), color purity and the (X, Y) values are presented in Table 1. From Table 1 it shows the color purity percentage at excitation wavelength of 314 nm for studied solvents.

Table 1. CIE color coordinates with color purity of 2-FBME in studied solvents.

Solvents	λ_a (nm)	λ_e (nm)	Band gap E_g(eV)	CIE Coordinates		Color purity (%)
				x	y	
Chloroform	269	431	3.62	0.1553	0.0948	93.5
Chloromethane	267	429	3.54	0.1569	0.0932	92.9
Butanol	268	478	3.65	0.1630	0.2396	69.7
Ethanol	268	427	3.52	0.1554	0.1788	80.3
Propanol	267	477	3.55	0.3588	0.4123	21.6
Decanol	265	474	3.56	0.1984	0.2280	57.2
Methanol	265	473	3.57	0.1568	0.2920	71.1

CONCLUSION

In this present work we have reported the simpler method of synthesizing benzopyrane coumarin derivative. Experimental band gap of the compound was calculated from this we may conclude that the Eg is one of the important parameter for fabricating optoelectronic devices. The photoluminescence emission spectra showed a slight bathochromic shift (red shift) in the studied solvents, these red shifts are probably due to increase in the polarity of the solvents and suggesting that the involvement of photo induced intermolecular charge transfer (ICT) state. These duality nature of wavelengths in 2-FBME molecule in different solvents is due to solvation effect, this results shows a simple extraction of dye in different solvents can be used to produce the desired wavelength. The 2-FBME possesses high color purity, good CIE chromaticity coordinate and they would have potential application in organic light emitting devices, this simple method to produce the blue light as blue component can play important role. The calculated chromaticity coordinates for 2-FBME in chloroform are near to standard chromaticity for excellent blue color and thus are promising blue producers for WLED application.

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