Furan Based Electronic Materials for LED and Solar Cell Application

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Abstract— In the current report, two novel chalcone derivatives (E) 1-(furan-2-yl)-3-(4-bromophenyl) prop-2-en-1-one (2AF4B) and (E) 1-(furan-2-yl)-3-(4-nitrophenyl) prop-2-en-1-one (2AF4N) were synthesized and crystallized using slow evaporation technique. The grown single crystals were chemically characterized by FT-IR vibrational technique to confirm the functional groups. The grown 2AF4B and 2AF4N crystals are thermally stable up to 131.59 °C and 224 °C respectively. The grown single crystals are characterized for their mechanical hardness. The 2AF4B and 2AF4N crystals possess high optical transmittance in the entire visible region, the optical band gap was calculated for the 2AF4B and 2AF4N crystals, and it was found to be 3.48 and 3.55 eV respectively. The grown crystals have blue light emission property which is confirmed by photoluminescence studies. The mechanical hardness, thermal stability, and optical band gap and photoluminescence property of the novel organic materials reveal the potentiality in LED and solar cell fabrication.

Keywords—Photoluminescence, Optical band gap, LED, solar cell

I. INTRODUCTION

The nonlinear optical crystals having an ample amount space in the field of photonic device applications. Therefore currently a great deal of research has been performed in the field of photonics. Particularly organic crystals draw an attention in recent years towards optical sensing, optical data storage, LED, and solar cell [1,2]. The selection of material for photonic applications depends on their photoluminescence, mechanical, optical, and thermal properties such as harness, high melting point, thermal stability, photo emission, and wide optical transparency. Also, organic nonlinear optical materials are attracting a great deal of attention, as they have large optical susceptibilities, inherent ultrafast response, and high optical thresholds for laser power as compared with inorganic materials [3]. In this context, the organic chalcone materials are most advisable because their structure can be easily tailored to enhance their optical nonlinearly as a consequence of the delocalization of ‘π’ electrons in the structure [4]. Subsequently the search for appropriate novel organic NLO materials exhibiting an ensemble of photoluminescence, mechanical, optical, and thermal properties never ceased. Therefore last two decades a large number of organic chromophores were designed [5]. Among them, furan is one of the most extensively employed electron rich material for these systems being their excellent thermal stability, wide optical transparency in the visible region, photo physical and mechanical hardness [6]. Taking these theoretical features in mind, currently we designed two new furan based chromophores for photonic applications. Moreover, the chalcone derivatives with a π-conjugated system that provides a large charge transfer axis. Among many other substituents nitro and bromo groups seems to be a better candidate for the substitution due to their push-pull behavior in the molecular axis. Since, bromo and nitro substitution in furan based chalcone derivative with better nonlinear optical efficiency, a novel nitro and bromo substituted push-pull type chalcone derivatives; (E) 1-(furan-2-yl)-3-(4-nitrophenyl) prop-2-en-1-one (2AF4N) & (E) 1-(furan-2-yl)-3-(4-bromophenyl) prop-2-en-1-one (2AF4B) have been synthesized and characterized using various spectroscopic studies. In the current report, mechanical hardness, thermal, optical and photoluminescence properties have been carried out for the grown crystals.

II. EXPERIMENTAL METHOD

The 2AF4B and 2AF4N compounds were synthesized using Claisen-schmidt condensation reaction and single crystals were grown by adapting slow solution evaporation technique [3-5]. A 2-acetyl furan ketone (0.01mol) and 4 bromo benzaldehyde (0.01mol) were mixed in 40 ml of ethanol and stirred for one hour at ambient temperature. A 2-acetyl furan ketone (0.01mol) and 4 nitro benzaldehyde (0.01mol) were mixed in 40 ml of ethanol and stirred for one hour at room temperature. Then the resulting product was poured in to the cold water and the isolated raw product was filtered and washed with sterilized water and dried to obtain the organic chalcone material. The synthesized compound was dissolved in 50 ml acetone and the saturated solution was filtered to remove the unwanted suspended entities in the solution. The saturated solution in a beaker was kept for nucleation with tight covering at room temperature for single crystal growth using slow evaporation method.

III. CHARACTERIZATION

The synthesized chalcone derivatives are characterized to confirm the functional groups in the sample using FTIR vibrational spectroscopic method. The FT-IR vibrational spectrum was obtained using thermo Nicolet, Avatar 370 spectrometer in the measurement range 4000 - 400 cm⁻¹ with KBr pellet method. The recorded FTIR Spectra of 2AF4B and 2AF4N is shown in Fig.1. The data for thermal analysis was obtained using simultaneous TGA/DSC SDT Q600 V20.9 Build 20 thermal
The recorded FTIR Spectra of 2AF4B and 2AF4N is shown in Fig.1. The characteristic peaks in the FTIR spectra at vibrational frequency between 3127 - 3008 cm\(^{-1}\) are attributed to aromatic C-H stretching vibrations in both the sample [7]. The vibrational band at 1645 cm\(^{-1}\) in the spectra is due to C=O stretching vibrations. The characteristic peak around 1600 cm\(^{-1}\) is assigned to C=C stretching vibrations. The vibrational frequency at 1253 cm\(^{-1}\) in the spectra is corresponding to C-O stretching vibrations. In the present study, C-C-C in plane bending vibrations is observed in the spectra at 868 and 775 cm\(^{-1}\). These respective vibrations in the FTIR spectra confirm the presence of functional groups in the synthesized chalcone derivative.

The simultaneous TG/DTA/DSC curves of 2AF4B and 4AF4N crystals are shown in Fig.2 and Fig.3. The sharp peak in the DSC curve shows good crystallinity and purity of the crystal. The smooth curve in DSC plot up to melting point is noticed from the microhardness analysis that the hardness number was found to be 11.59 kg/mm\(^{2}\) and 12.33 kg/mm\(^{2}\) for 2AF4B and 2AF4N respectively. The obtained hardness number is better than that of standard urea (6-11 kg/mm\(^{2}\)). Therefore the grown crystals are capable candidates in device fabrications.

V. CONCLUSION

A furan based organic single crystals were grown by slow evaporation technique. FTIR studies confirm the functional groups in the sample. The mechanical hardness was estimated using Vickers microhardness test on a well-defined plane of the crystal. Indentations were made for varying load and average of the diagonal length was used to estimate the microhardness of the crystal. The Vickers microhardness was calculated under the relation \(H_v = \frac{1.8544 P/d^2}{\text{kg/mm}^2}\) [11] where, \(P\) is the applied load in kg, \(d^2\) is the average diagonal length of the indenter impression in mm. It is noticed from the microhardness analysis that the hardness number increase with respect to the increase of ‘P’ and remains unchanged. The hardness number is found to be 11.59 kg/mm\(^{2}\) and 12.33 kg/mm\(^{2}\) for 2AF4B and 2AF4N respectively. The obtained hardness number is better than that of standard urea (6-11 kg/mm\(^{2}\)). Therefore the grown crystals are good material for LED and solar cell applications.

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Fig.1. The FT-IR vibrational spectra of 2AF4B and 2AF4N crystals

Fig.2. The TG/DTA/DSC Curve of 2AF4B crystal

Fig.3. The TG/DTA/DSC Curve of 2AF4N crystal

Fig.4. The UV-Visible spectra of 2AF4B crystal

Fig.5. The UV-Visible spectra of 2AF4N crystal
REFERENCE


