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 ^{0}C and 224 ^{0}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 nonlinearity 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-schimidt 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

analyzer under nitrogen gas flow with a heating rate of 10 ^{0}C min^{-1} on sample in the temperature range between 25 ^{o}C and 600 ^{o}C. The simultaneous TG/DTA/DSC curve of 2AF4B and 2AF4N crystal is shown in **Fig.2 and Fig.3**.

The linear optical properties have been analyzed with the help of UV-Vis-NIR spectrum. The spectral data was collected for the sample using Shimadzu 1800 UV-Vis-NIR spectrophotometer in DMF solution (0.01mol) in the wavelength range 200 -1100 nm at room temperature. Vickers microhardness tester (CLEMEX digital micro hardness tester "MATSUZAWA", Japan) was used to study the mechanical properties of the crystals. The photoluminescence (PL) data was recorded between 400nm and 600nm by using FluoroMax-4CP spectrometer at room temperature with an excitation wavelength 350 nm.

IV. RESULTS AND DESCUSION

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 line 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 indicates the toughness of the crystal against thermal crack. There is no endothermic or exothermic peaks are appeared in the DSC/DTA curve after melting point. The thermal resistance of 2AF4B and 4AF4N endures superior than that of standard urea (130 ^{o}C) [4] and don't get decomposed till their melting point 131.59 and 224 ^{0}C respectively. Thus, the analysis report suggests that the 2AF4B and 2AF4N crystals are advisable material for LED and solar cell applications up to its melting temperature.

The optical transparency in the visible region is very essential factor for an NLO crystal to be useful in NLO applications. The UV-Visible spectrum of the crystal was shown in **Fig.4 and Fig 5**. The recorded spectra reveals that the 2AF4B and 2AF4N crystals have a wider transparency range extending into entire visible and infrared region and the absorption is noticed in the UV region at 323 and 319 nm respectively this may be oriented in consequence n-π* transitions. [8]. The cut-off wavelength for the crystal 2AF4B and 2AF4N is found to be 366 and 383 nm respectively.

The optical band gap (E_g) of the crystal using Tauc's equation [9], $(\alpha h\vartheta) = \alpha_0(h\vartheta - E_g)^n$.

Where, 'α' is the linear absorption coefficient, 'α_0' is the band edge constant that depends on the transition probability, and 'n' is the index that characterizes the absorption process; theoretically the value of n can be given by ½ and 2 for direct and indirect band gap structure respectively. The direct band gap can be estimated by plotting a graph (hν) v/s $(\alpha h\vartheta)^2$ and shown in **Fig.6 and Fig.7**. The band gap (E_g) can be determined from extrapolating the linear portion of the curve to a point $(\alpha h\vartheta)^2 = 0$ and the direct band gap value thus obtained is 3.48 eV and 3.55 eV for 2AF4B and 2AF4N respectively. Hence, the 2AF4B 2AF4N crystals can be a potential material for LED and solar cell applications.

The photoluminescence spectrum has recorded **(Fig.8)** at room temperature with an excitation wavelength 350nm. The emission spectrum shows a strong emission peak at 493 and 491 nm for 2AF4B and 2AF4N respectively. The peaks correspond to blue region (493nm and 491 nm). The defect states in blue region have blue light emission properties, which can be used for blue LED applications [10].

The mechanical strength of the grown crystal was characterized by 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= 1.8544 P/d^2 kg/mm^2 [11] where, P is the applied load in kg, 'd' 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 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 hardness test and hardness number was found to be 11.59 kg/mm^2 and 12.33 kg/mm^2 for 2AF4B and 2AF4N respectively. The thermal study (TG/DTA/DSC) confirms the material stability up to their melting point (131.59 and 224 ^{o}C). The noticed optical band gap (3.48 and 3.54 eV) and high transparency range beyond the cut-off (383 and 366 nm) in the curve indicates that the grown crystals are suitable for nonlinear optical device fabrications. The photoluminescence peak (at 493 and 491 nm 2AF4B and 2AF4N respectively) shows the blue light emissions in the visible region. It can be concluded that the grown crystals are good material for NLO applications.

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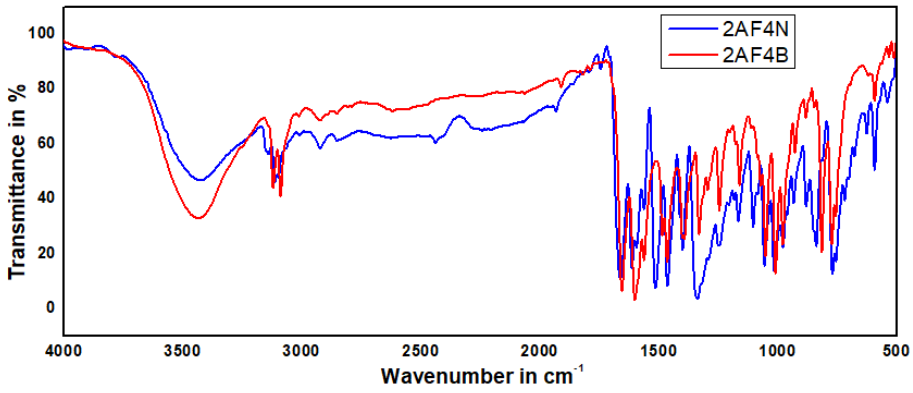
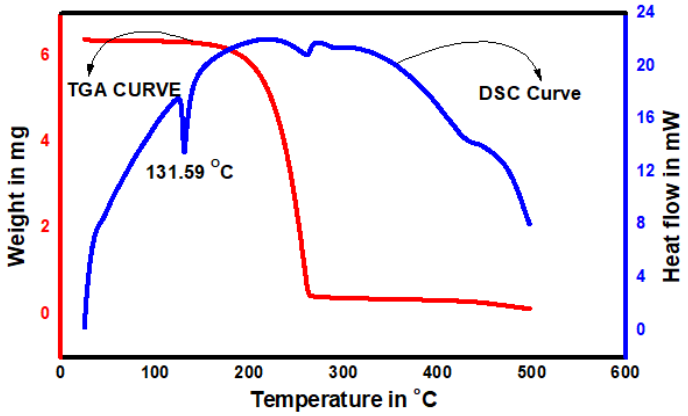


Fig.1. The FT-IR vibrational spectra of 2AF4B and 2AF4N crystals



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

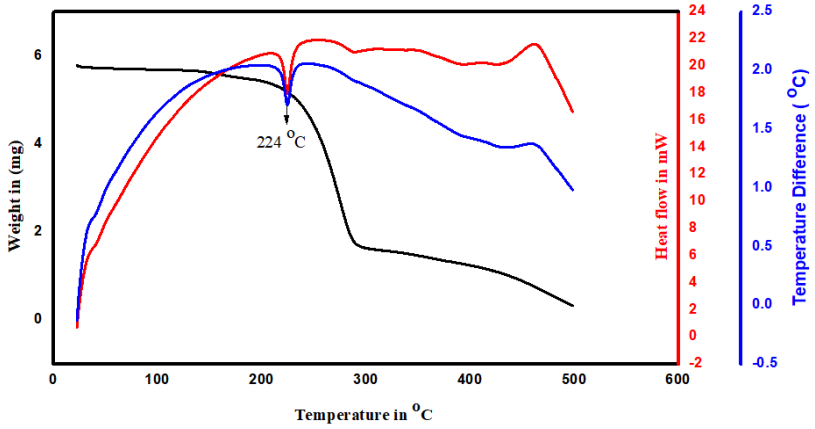


Fig.3. The TG/DTA/DSC Curve of 2AF4N crystal

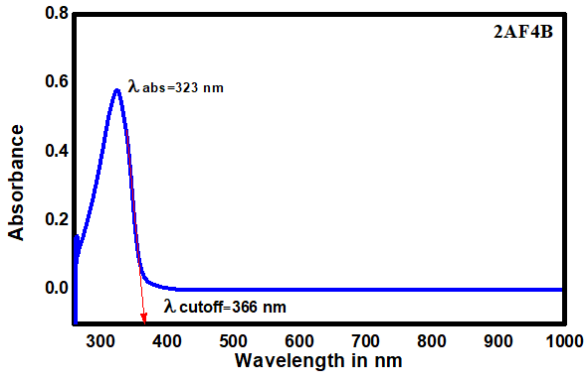


Fig.4. The UV-Visible spectra of 2AF4B crystal

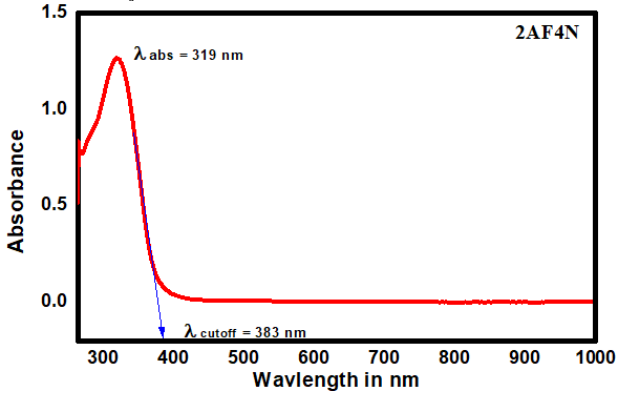


Fig.5. The UV-Visible spectra of 2AF4N crystal

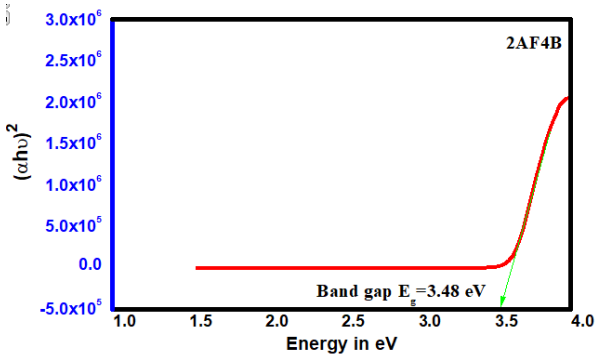


Fig.6. Optical band gap of 2AF4B crystal

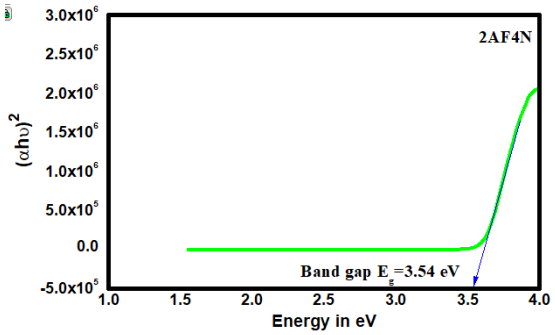


Fig.7. Optical band gap of 2AF4N crystal

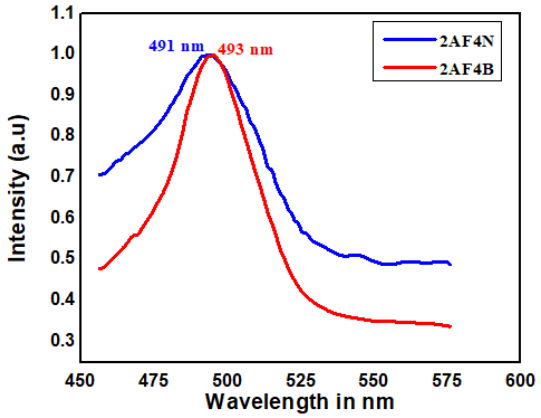


Fig.8. Photoluminescence spectra of 2AF4B and 2AF4N Crystals

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