International Journal of Physics and Applications.
ISSN 0974-3103 Volume 9, Number 1 (2017), pp. 25-31

http://www.irphouse.com

NLO AND OPTICAL PROPERTY OF NEWLY SYNTHESIZED CHALCONE COMPOUND (2*E*)-1-(4'-BROMOBIPHENYL-4-YL)-3-(3-BROMO-4-METHOXYPHENYLL)PROP-2-EN-1-ONE

Vinutha P R[1], Jayarama A[2], Kaliprasad C S[3], Narayana Y[3] and Suresh Kumar M R[4]

[1] Dept. of Physics, Bearys Institute of Technology, Innoli, Mangalore
[2] Dept. of Physics, Sahyadri College of Engineering and Management, Mangalore
[3] Dept. of Physics, Mangalore University, Mangalagangotri
[4] Dept. of Physics, Alliance University, Bengaluru
**Corresponding author*

Abstract

The title compound (2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(3-bromo-4-methoxyphenyll)prop-2-en-1-one (BDCP) was synthesized using 4'-(4-bromophenyl) acetophenone and 3-bromo-4-methoxy benzaldehyde in 1:2 ratio. The NLO, crystalline and optical property of newly synthesized chalcone compound was characterized by SHG, powder XRD, FTIR and UV-Visible spectroscopy. The second harmonic generation (SHG) efficiency of the chalcone crystal was found to be 1.26 times that of urea. This is a strong second harmonic generation (SHG) efficiency among chalcone derivatives. The UV-VIS spectrum shows a cut-off wavelength at 430 nm. The crystal has strong absorption band in the UV region. In the present study the crystallinity of the chalcones was confirmed using powder XRD method.

1. INTRODUCTION

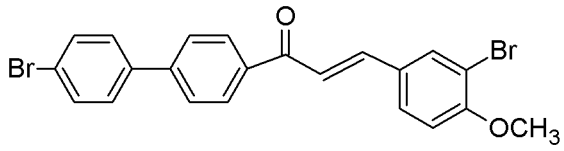
The design and synthesis of organic molecules exhibiting nonlinear optical (NLO) properties have been motivated by their potential for applications in optical communications, optical computing, data storage, dynamic holography, harmonic generators, frequency mixing and optical switching [1-2]. Organic materials are of particular interest because of their versatile synthetic flexibility that offers one to fine

tune the optical properties at molecular level. Moreover, the optical nonlinearity in this class of materials is electronic in origin and hence exhibits an ultra fast response. Chalcones are a family of cross conjugated NLO chromophores that exhibit good SHG efficiency and transparency [3-5]. By suitably selecting the molecular components, it is possible to fine tune the physico-chemical properties of chalcones. The objective of the present work is to synthesize the chalcone derivative (2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(3-bromo-4-methoxyphenyll)prop-2-en-1-one and its characterization by FTIR, UV-Vis spectroscopy, SHG and XRD studies, to confirm the crystallinity and optical property of the compound.

2. MATERIALS AND METHODS

A Synthesis of Crystal

The Claisen–Schmidt condensation reaction is one of the well established method to synthesized the chalcone derivative. The required chalcone (2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(3-bromo-4-methoxyphenyll)prop-2-en-1-one were synthesized by aldol condensation of equimolar quantities of 4'-(4-bromophenyl)acetophenone with 3-bromo-4-methoxy benzaldehyde using methanol as solvent [6]. The reaction was conducted at room temperature with gradual mixing of NaOH solution and it was monitored using thin layer chromatography. The reaction mixture is poured on to 250g of crushed ice with vigorous stirring. The precipitate formed was filtered, dried and recrystalized from ethanol. A white slimy product is obtained which upon refrigerating overnight yielded a white powdery product. The good quality single crystals of BDCP was grown using acetone as solvent at room temperature.



(2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(3-bromo-4-methoxyphenyl)prop-2-en-1-one

Figure 1. Synthesis of Title compound.

B. Characterization of Compound

The mass of the title compound was measured by using LCMS-8050 Triple Quadrupole Liquid Chromatograph Mass Spectrometer (LC-MS/MS). Kurtz and Perry developed the technique to measure the SHG intensity of the crystals [7]. The crystal was powdered and densely packed in a capillary. An Nd: YAG laser beam of wavelength 1064 nm, pulse width 8ns and repetition rate 10 Hz was made to fall normally on the sample in the capillary tube. The second harmonic signal was

detected by a photo multiplier tube (Hamamatsu R2059) and displayed on a storage oscilloscope Tektronix (TDS 3052B). The UV-Visible absorption spectrum of the crystal was recorded using a UV-1800 SHIMADZU UV-Visible spectrophotometer in the wavelength range of 200-800 nm.

FTIR spectrum is used to analyze the presence of functional groups in the newly synthesized BDCP crystal. The FTIR spectrum was recorded in the region 400 to 4000 cm^{-1} using the NICOLET 6700, USA spectrometer. The sample used was mixed with known amount of KBr to make pellet. The characteristic absorption peaks are observed in the range from 400 to 4000 cm^{-1}. Differential thermal (DT)/thermogravimetric (TG) analysis were carried out on the NBG samples to look for possible phase transitions and to determine the melting point. TG/DTA studies for NBG were made using Universal V4.5A TA Thermal analyzer at a heating rate of 10 $^0C\ min^{-1}$ under nitrogen atmosphere. Powder X-ray diffraction data was collected for the title compound using Rigaku X-ray diffractometer with CuKα radiation (l = 1.5405 A°) with an applied operating voltage 30 kV and current 20 mA. The sample in the form of powder was mixed with binder and smeared on the surface of a glass slide. The sample was mounted on the centre of a diffractometer table.

3. RESULTS AND DISCUSSION

The mass spectrum is a record of relative ion abundance versus m/z as shown in Figure 2. The measured value (m/z = 472.85) of title compound is nearly equal to the theoretically calculated mass 472.17. Therefore the synthesis of the compound was confirmed. The SHG efficiency of newly grown crystal is presented in Table 1. The KDP was used as reference material to measure the SHG efficiency. SHG conversion of the newly grown crystal was found to1.26 times that of Urea and 12.6 times that of KDP. Normally the non-centrosymmetric structured compounds show the high SHG value. The reported results shows that bromine attached to the benzene ring improves the donor acceptor group which is responsible for SHG conversion efficiency of the material [8-10]. This is also one of the reason for increase in SHG conversion efficiency of the Title compound.

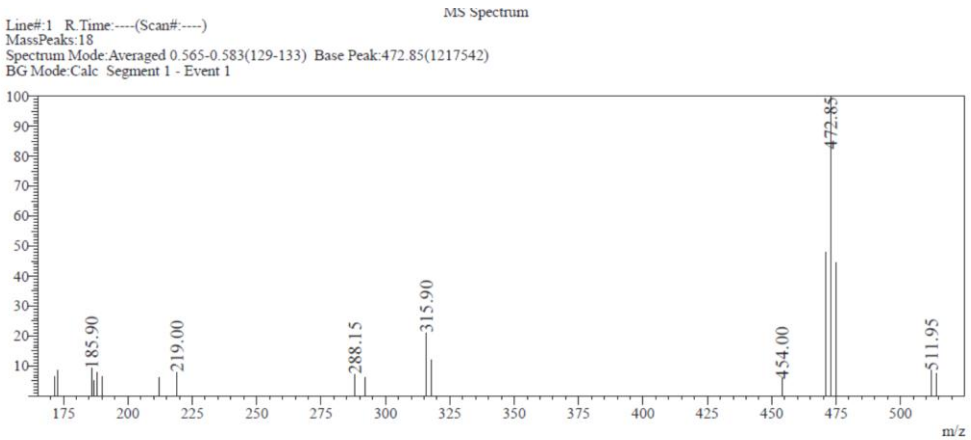


Figure 2. Mass spectrum

Table 1. SHG efficiency of the title compound.

Name of the compound	SHG efficiency (Urea = 1)
((2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(3-bromo-4-methoxyphenyll)prop-2-en-1-one (title compound)	**1.26**
Potassium di phosphate (KDP)	0.1

The characteristic absorption peaks are observed in the range from 400 to 4000 cm^{-1} is shown in Fig.3. The title compound shows the strong bond at 3053 cm^{-1} due to the aromatic C-H stretching [11]. The wave number at 1676 cm^{-1} attributable to the C=O stretch, Which confirms the formation of chalcone. The obtained frequencies at 1600 to 1571 cm^{-1} is considered to be a C-C stretching. The band region 1222 cm^{-1} is to be C-N Vibrations. The C-O stretching observed in the band region of 1074 to 1010 cm^{-1} in FTIR. The band at 657 to 443 cm^{-1} in FTIR are due to C-H out of plane deformation/C-C==O deformation. Thus the FTIR spectral confirms the presence of the functional groups and their mode of vibrations.

The UV-visible spectrum of the title compound is shown in Figure 4. The graph shows the lower cut-off at 430 nm, it is transparent at the visible region. In the UV-region, the crsytal have strong absorption band, which can be used for NLO applications at room temperature. The Chalcones are normally absorb UV light due to the excitation of unpaired electrons. The thermal analysis was carried out in the temperature range between 30 ^{0}C and 700 ^{0}C and the response curve of BDCP sample is shown in Fig. 5. The DTA curve shows a major endothermic peak, which corresponds to the melting point of the material at 120 ^{0}C and it shows exothermic peak at 560 ^{0}C, after that the compound decomposes. The BDCP compound shows decomposition between 200 ^{0}C to 300 ^{0}C with a maximum weight loss of 76%.

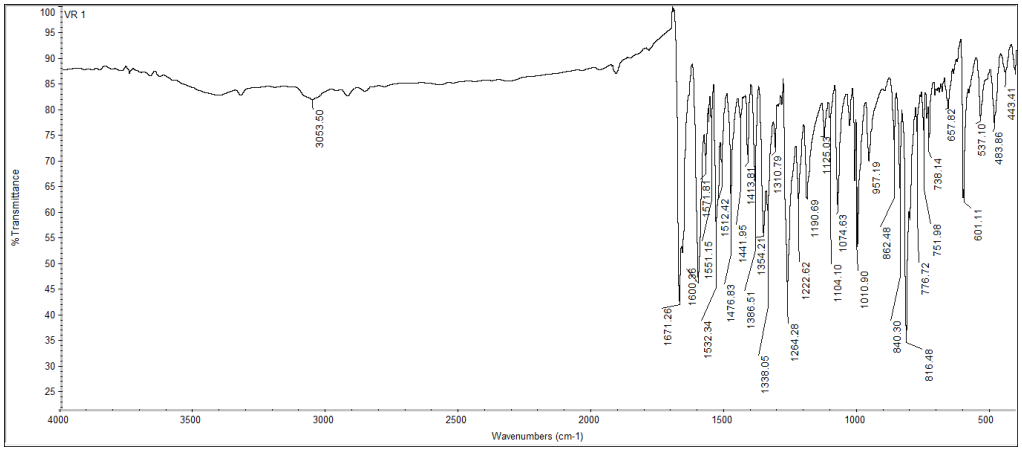


Figure 3. FTIR spectrum of BDCP crystal.

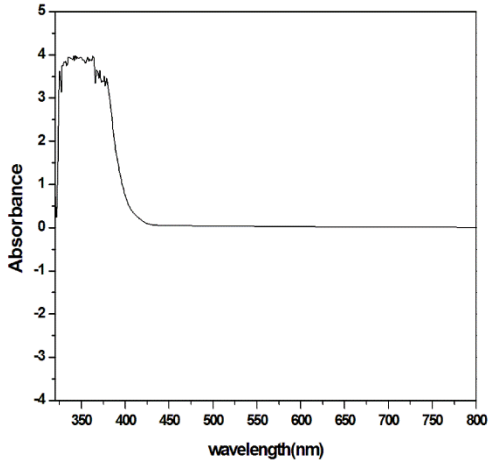


Figure 4. UV absorption spectra

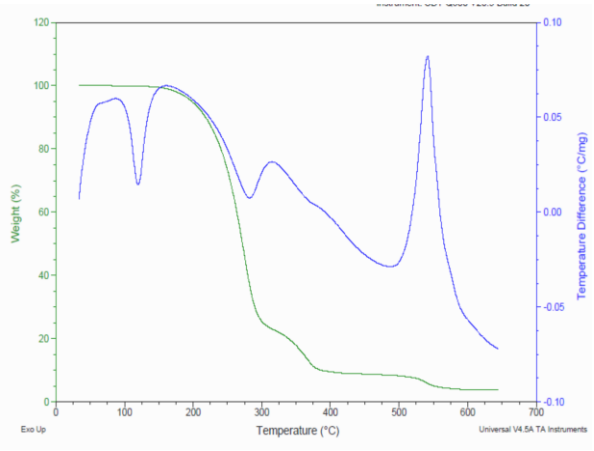


Figure 5. TG and DTA curves of BDCP.

The X-ray powder diffraction analysis was carried out using Rigaku X-ray diffractometer and the sample was scanned over 2θ range from 10^0 to 70^0 at a range of 2^0 per minute. The obtained spectrum is shown in Figure 6. The lattice parameters of the all the compounds are calculated and summarized in Table 2. The spectra shows many sharp peaks and the sharp peaks indicate that these are highly crystalline in nature. From the recorded X-ray diffraction the peaks corresponding to (111) has a maximum counts 5250 and it is more intense peak in the pattern.
The maximum number of hkl values 110 indicates the BCC crystal.

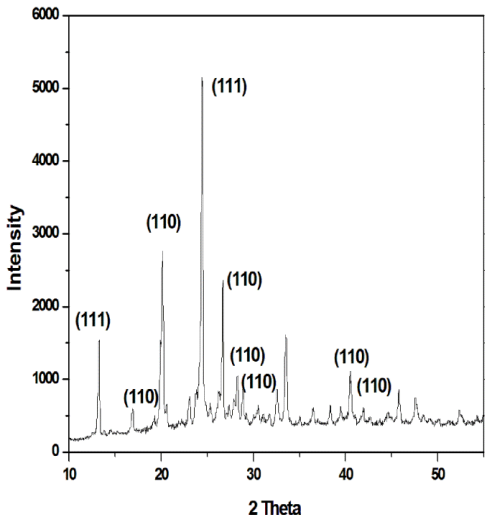


Figure 6. Powder diffraction spectrum

Table 2. Powder XRD data for BDCP

Theta	intensity (cps)	d	hkl	Q
13.30	1540.00	0.027616	111	2.923904
16.90	601.00	0.063723	110	6.746963
20.20	2760.00	0.0481	110	5.095993
24.40	5250.00	0.0276	111	2.920524
26.70	2360.00	0.054351	110	5.754601
28.30	1050.00	0.076994	110	8.151996
29.20	537.00	0.068899	110	7.294935
30.50	641.00	0.034043	111	3.604475
38.00	419.00	0.011541	112	1.221899
38.30	640.00	0.022788	111	2.412737
40.50	1110.00	0.075885	110	8.034659
41.90	609.00	0.06645	110	7.035631
42.60	483.00	0.049082	110	5.196695
51.10	436.00	0.031205	122	3.303917

4. CONCLUSION

The title compound BDCP was synthesized by using the Claisen–Schmidt condensation reaction method and the synthesis was confirmed by mass analysis and FTIR. The FTIR confirms the functional group presence in the synthesized compound. Powder X-ray diffraction studies were carried out to confirm the crystalline nature of compound and lattice parameters values hkl were calculated and Q values were derived. The SHG and UV measurements show that the title compound has good NLO property as compared to urea and KDP, and it has a strong absorption band in the UV-region.

REFERENCE

[1] Chemla, D.S., Zyss, J., 1987, Nonlinear Optical Properties of Organic Molecules and Crystals, Academic Press, New York.

[2] Prasad, P.N., Williams, D.J., 1991, Introduction to Nonlinear Optical Effects in Organic molecules and Polymers, Wiley, New York.

[3] Ravindra, H.J., Kiran, A.J., Satheesh, R.N., Dharmaprakash, S.M., Chandrasekharan, K., Balakrishna, K., Rotermund,F., 2008, J. Cryst.Growth., 310,pp- 2543

[4] Kiran, A.J., Kim, H.C., Kim, K., Rotermund, F., Ravindra, H.J., Dharmaprakash, S.M., Lim, H., 2008, Appl. Phys. Lett., 92, pp-113307

[5] Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A., Watanabe, Y., 1988, Mol. Cryst. Liq. Cryst. 315, PP-135

[6] Prabhu, A.N., Jayarama,A., Bhat, K.S., and Upadhyaya, V., 2013. J Mol Str., 1031, pp-79-84.

[7] Kurtz, S.K., Perry, T.T., 1968, J.Appl.Phys., 39, pp-3798.

[8] Navin, N. Bappalige., Narayana, Y., Boja Poojary and Narayana Poojary, K., 2010, Journal of Pure and Applied Physics. 6, pp-151-156.

[9] Kitazawa, M., Higuchi, R., Takahashi, M., wada, T., and Sasabe, H., 1994, Appl.Phys Lett.64, 2477.

[10] Endoh, H., Kawaharada, M., and Hasegawa, E,. 1996, Appl.Phys.Lett.68, 293.

[11] Socrates, G., 1980, Infrared Characteristic Group Frequencies, Wiley, New York,