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Growth and characterisation of 2′, 3, 4, 4′, 5-Pentamethoxychalcone (PMC) – For non linear optical applications

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ABSTRACT

An organic NLO crystal, 2′, 3, 4, 4′, 5-Pentamethoxychalcone (PMC) with a dimension of 13 × 10 × 3 mm^3 was grown by slow evaporation method. The cell parameters of PMC crystal was confirmed by Powder X-ray diffraction. FTIR and FTRaman spectroscopy were used for the identification of functional groups for the various modes of vibrations. The UV cut off range has been determined by using optical absorption study. Thermal stability of the grown crystal has been analysed by TG-DTA studies. Factor group analysis and Dielectric studies were also carried out. Photoluminescence study was performed for PMC. The first order hyperpolarizibility and HOMO–LUMO analysis were performed using DFT calculations using Gaussian 03 software. Non linear optical (NLO) behaviour of PMC crystals is studied by using Kurtz & Perry powder Technique and SHG efficiency has been found 2.02 times higher than that of KDP.

1. Introduction

Nonlinear optical materials are the active elements for optical communications and optical electronics. Among such NLO materials, organic materials are shown to be superior and have distinguishing features to their inorganic counter parts in terms of synthesis, crystal fabrication, much faster optical nonlinearities, tailorability of designing new crystals with high optical quality, cost effective, processability, high damage threshold and ease of fabrication into desired shapes [1,2]. The second-order nonlinear optical property of organic compound is derived from conjugated delocalized π electrons and intermolecular interaction.

In the synthesis of many pharmaceuticals, chalcones are important intermediates and in material fields chalcones have high attention in potential applications such as Non-Linear Optical (NLO), Optical Limiting, and Electrochemical sensing [3]. In recent years, Chalcone NLO crystals and its derivatives have very high deal of attraction to their large optical nonlinearities [4,5]. Chalcone derivatives with a suitable electron donor and acceptor substituent are one among the efficient organic NLO materials. The members of α, β-unsaturated ketones (Chalcones) and flavonid family have attracted a great deal of interest due to their potential applications in Non Linear Optics due to high second harmonic generation efficiency and have high values than Urea [6]. α, β-unsaturated ketones are commonly synthesized via the Claisen–Schmidt condensation. This reaction is catalyzed by acids and bases condition. In chalcone chromophores asymmetric electronic distribution in either or both ground and excited states enhanced by substitution of suitable electron donor or acceptor group like OCH_3, leading to an increased optical nonlinearity [7]. Chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. In this paper we are reporting the Growth, FTIR, FTRamam, Photoluminescence and dielectric studies of 2′, 3, 4, 4′, 5-Pentamethoxychalcone (PMC).

2. Experimental

The 2′, 3, 4, 4′, 5-Pentamethoxychalcone (PMC) were prepared by using the Claisen–Schmidt condensation method. Commercially available of 2′, 4′-dimethoxyacetophenone (Sigma-Aldrich) and 3, 4, 5-trimethoxybenzaldehyde (Sigma) have been procured and used. Here, 0.01 mol of 2′, 4′-dimethoxyacetophenone was mixed with 0.01 mol of 3, 4, 5-trimethoxybenzaldehyde in N,N-Dimethylformamide (DMF) (20 ml) and the mixture was treated with an aqueous solution of potassium hydroxide (2 ml, 30%). This mixture was stirred well and kept aside for 24 h. The resulting solid mass was collected by filtration and dried. Solubility study was

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carried out and DMF is found that suitable solvent for the crystal growth of PMC. The obtained compound was purified three to four times by re-crystallizing in DMF. Optically clear and well defined crystals were harvested after a span of some days with a dimension of 13 × 10 × 3 mm^3. The schematic representation of the reaction and solubility curve of PMC is given in Fig. 1. Grown crystal and morphology of PMC is shown in Fig. 2.

3. X-ray diffraction analysis

The grown crystals were characterized by Powder X-ray Diffraction (XRD) analysis by using BRUKER, GERMANY (D8 Advance) X-ray diffractometer with Cu Kα radiation. The scanning rate of sample was in the range of 10–80°. The powder X-ray diffraction pattern of PMC is shown in Fig. 3. All intensity peaks could be indexted and the lattice parameter values of PMC were calculated from X-Ray Powder Diffraction data using XRDA

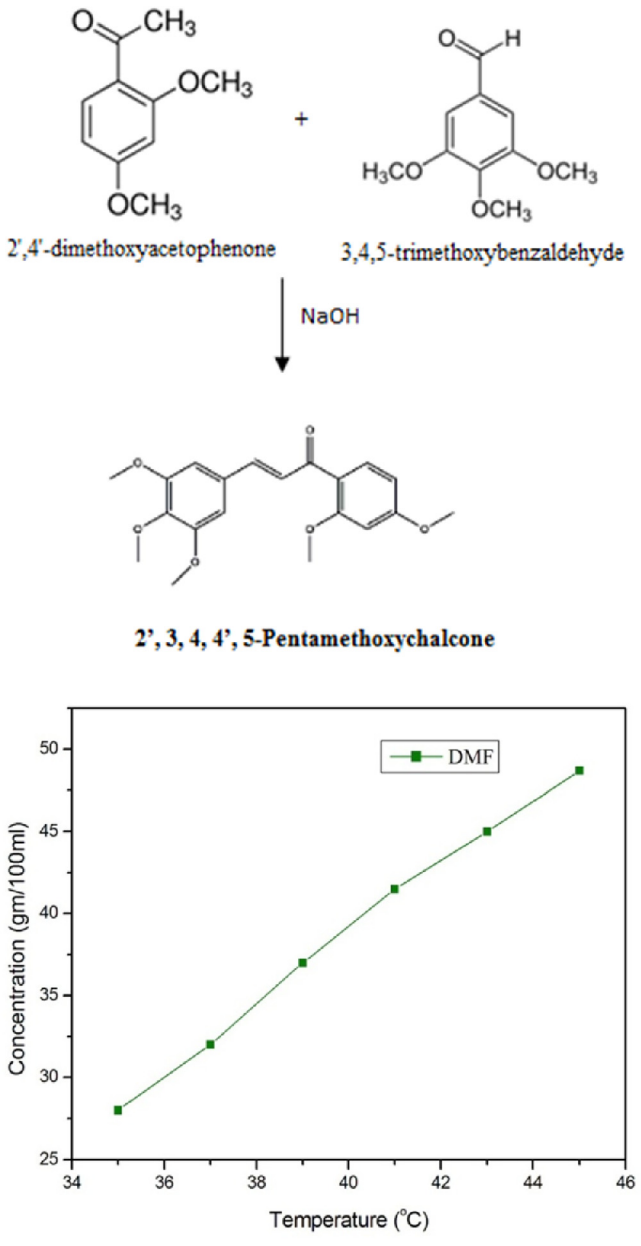
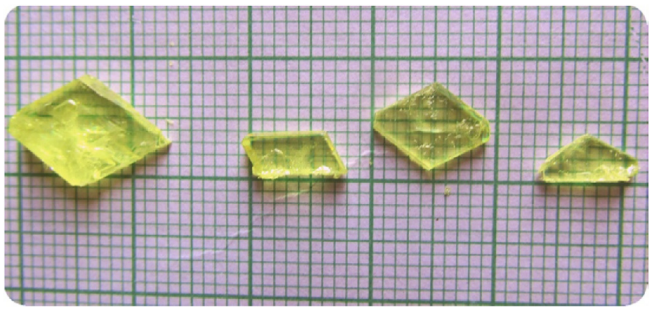


Fig. 1. Reaction mechanism and solubility curve of PMC Scheme.



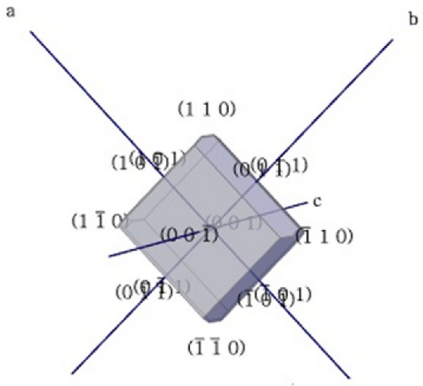


Fig. 2. As grown crystals and morphology of PMC

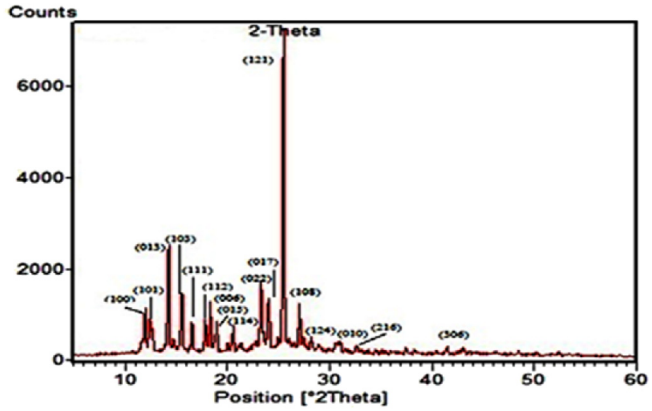


Fig. 3. Powder diffraction pattern of PMC

software. Grown crystal structure is found to be Orthorhombic crystal structure system and it belongs to $P2_12_12_1$ Space group. The obtained lattice parameter values are depicted in table (1) which is in good agreement with the literature value [8] (see Table 1).

4. Vibrational analysis of PMC

4.1. Factor group analysis of PMC

The factor group analysis was performed for the title compound by following the procedures outlined by Rousseau et al. [9]. The symmetry properties of crystal is determined by the factor group analysis by studying the effect of the symmetry opterations of the factors group on each type of atom in the unit cell [10]. The vibrational spectral studies provide information about the charge