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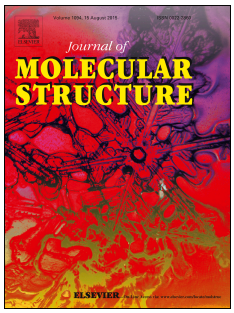

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Crystal growth and characterization of new nonlinear optical Piperidine derivative: (4-hydroxypiperidin-1-yl)(4-methylphenyl) methanone

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Abstract

Organic compound (4-hydroxypiperidin-1-yl)(4-methylphenyl)methanone[HPMP] with molecular formula $C_{13}H_{17}N\,O_2$ was synthesized using Scholten-Boumann condensation reaction method. The single crystals were grown using slow evaporation solution growth technique. Single crystal XRD study shows that the compound crystallizes in the orthorhombic system with a space group $Pca2_1$. ^1H and ^{13}C-NMR spectra were recorded to identify the various types of protons and carbons present in the compound and confirm the chemical structure. The Various functional groups present in the compound were identified using recorded FT-IR spectrum. The UV–Visible spectrum study reveals that the crystal is transparent in the entire visible region and the absorption is observed at 236 nm. The PL spectrum shows the emission takes place at 432 nm. The thermal study reveals that the thermal stability of the crystal is good. The Kurtz powder second harmonic generation (SHG) test shows that the HPMP is NLO active and its SHG efficiency is 1.86 times that of KDP. The micro hardness test was carried out and the work hardening coefficient value (n) of the crystal was found to be 2.20. This indicates that the crystal is hard and is suitable for device application.

Keywords: Piperidine; Crystal growth; Non-centrosymmeric; Second harmonic generation efficiency; Single crystal XRD; ^{13}C-NMR;^{1}H-NMR; FT-IR; UV-Visible; Photoluminescence studies; TG/DTA; Vicker's micro hardness.

1. Introduction

Engineering of new nonlinear materials, both organic and inorganic, structures and devices with enhanced figures of merit has comported over the past two decades as a major force to drive nonlinear optics from the laboratory to real applications. There is currently a considerable effort to develop new organic materials with large second-order nonlinear optical (NLO) susceptibilities because of their potential applications in optical signal processing and frequency conversion [1–5].

The nonlinear optical (NLO) properties of molecules and their hyperpolarizabilities have become an important area of extensive research, and a lot of experimental and theoretical efforts are focused on bulk NLO properties (like second order and third orders harmonics) as well as their dependence on the hyperpolarizabilities (β and γ) of molecules. Currently much attention has been given to organic NLO materials because of their large first (β) and second (γ)