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Short Communication

Structural and spectral characterization of novel non-centrosymmetric 2,4-dinitrobenzene derivative

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HIGHLIGHTS

- A novel organic nonlinear optical material DNPAP has been synthesized.
- It has good physicochemical properties suitable for second harmonic generation.
- The SHG efficiency of DNPAP is found to be 6.4 times better than that of KDP.

GRAPHICAL ABSTRACT



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ABSTRACT

A novel organic compound 9-(2,4-dinitrophenyloxy)-3,3,8-trimethyl-1,5-dihydro-[1,3]dioxepino [5,6-c]pyridine (DNPAP) has been synthesized and a nonlinear optical (NLO) crystal has been grown by slow evaporation method. Compound was subjected to different characterization analyses in order to find out its suitability for optoelectronic applications. Single crystal and powder X-ray diffraction analyses show that DNPAP crystallizes in the orthorhombic space group $Pca2_1$. The range of optical absorption was ascertained by recording UV–Vis spectrum. The second harmonic generation (SHG) test has shown that DNPAP possesses 6.4-times higher NLO efficiency compared to KDP.

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Introduction

Development and research of new nonlinear optical (NLO) materials is an important problem in modern materials science [1,2]. Currently, many inorganic crystals, such as quartz, potassium and ammonium dihydrophosphates, lithium niobate, potassium

titanyl phosphate, have been developed and introduced into the practice. Despite the fact that only a limited number of non-linear optical materials based on organic compounds have been applied in the industry [3], this area is an active field of research. Organic single crystals possess unique optoelectronic properties because organic molecules have delocalized electrons which exhibit various photoresponses such as photoconductive, photovoltaic, and photocatalytic behavior [4]. Organic NLO materials offer in fact, as compared to traditional inorganic ones, some appealing features as lower dielectric constants, higher theoretically achievable EO

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