Materials Chemistry and Physics 312 (2024) 128662

Contents lists available at ScienceDirect

Materials Chemistry and Physics

journal homepage: www.elsevier.com/locate/matchemphys

Enhancing nonlinear optical responses via Methoxy Positional Isomerism in Chalcone-Based Materials

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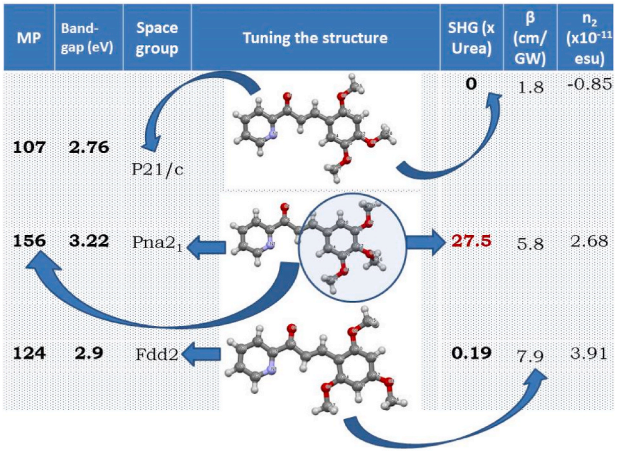
HIGHLIGHTS

- PTMP2 demonstrates enhanced thermal stability, indicating its potential as a stable nonlinear optical material.
- Crystallographic analysis reveals non-centrosymmetric space group, favoring NLO applications in PTMP derivatives.
- Methoxy substitutions correlate with increased melting points, reflecting phenylene moiety's enhanced donor strength.
- Chalcone derivatives exhibit high transparency, wide energy band gaps, and varying third-order NLO properties.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:
Chalcones
Z-scan
2-Acetylpyridine
SHG
Nonlinear optical

ABSTRACT

The functional moieties present in chalcone derivatives play a pivotal role in finely adjusting the thermal, optical, structural, and nonlinear optical (NLO) characteristics of the chalcone material. This paper details the synthesis of chalcone derivatives where three distinct trimethoxy substituents are integrated into the benzoyl moiety through carboxyl bonding with 2-acetyl pyridine. The synthesis employs the Schmidt condensation method, and the resultant samples are subject to scrutiny through FTIR and FT-Raman techniques to ascertain phase purity. The outcomes reveal substantial alterations in the structural, thermal, optical, and NLO attributes of the samples. The electron-donating property of the trimethoxy groups augments electron density within the chalcone molecule, thereby effecting multiple shifts in the material's characteristics. Interestingly, a methoxy group located at

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https://doi.org/10.1016/j.matchemphys.2023.128662
Received 17 September 2023; Received in revised form 27 October 2023; Accepted 5 November 2023
Available online 13 November 2023

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