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An experimental and theoretical study on a novel donor-π-acceptor bridge type 2, 4, 5-Trimethoxy-4′-chlorochalcone for optoelectronic applications: A dual approach

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Abstract

In this article the authors aim is to investigate and analyze the various key parameters of a organic D-π-A type novel nonlinear optical material 2, 4, 5-Trimethoxy-4′-chlorochalcone (2,4,5TMCC) through experimental and quantum chemical studies. The Claisen–Schmidt condensation reaction mechanism was applied to synthesize the 2,4,5-TMCC compound and its single crystal was grown by a slow evaporation solution growth (low cost) technique. The crystal structural was confirmed by powder X-ray diffraction analysis. The robust vibrational study has been done using FT-IR and FT-Raman spectra and its NLO activity has been discussed. The factor group analysis was also performed. The optical absorption spectrum was recorded and the band gap was calculated to be 2.8 eV. In Photoluminescence spectrum, an intense emission band at ~540 nm has been observed which shows that the grown crystals can be used in green organic light emitting diodes and laser applications. To achieve the stable ground state molecular geometry of 2,4,5TMCC, the computational techniques were applied at different levels of theory using 6-31G* basis set. The calculated geometrical parameters and vibrational spectra are found to be in good agreement with the experimental results. To probe the optical properties of the title compound the time dependent density functional theory has been applied. The excitation wavelength was observed at ~398.63 nm calculated at B3LYP/6-31G* level of theory and found