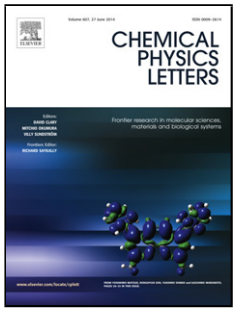

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Synthesis, Single crystal structure, Hirshfeld surface and Theoretical investigations on pyrimidine derivative

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Abstract

Nonlinear optical organic crystal of ethyl-6-(chloromethyl)-4-(4-hydroxy-3-methoxyphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylatemonohydrate (CHMTM) were grown by the slow evaporation technique. Structural characterization was made by X-ray diffraction method, further characterized by FT-IR, FT-Raman, and NMR spectra. The equilibrium geometry and harmonic vibrational wavenumbers were computed using Density Functional Theory (DFT) method. The vibrational assignments were carried out with the help of potential energy distribution (PED) analysis. The intermolecular interactions of the crystal structure were analysed using Hirshfeld surface and fingerprint analysis. Charge transfer analysed with the help of NBO analysis. The nonlinear optical properties (NLO) and energy gap (E_g) analysis were also investigated.

Keywords : CHMTM, Single crystal XRD, Hirshfeld surface, NLO, 2D-Fingerprint plot.

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